Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 02:27 pm GMT

PDB ID	:	7AIH
EMDB ID	:	EMD-11796
Title	:	The Large subunit of the Kinetoplastid mitochondrial ribosome
Authors	:	Soufari, H.; Waltz, F.; Parrot, C.; Bochler, A.; Hashem, Y.
Deposited on	:	2020-09-27
Resolution	:	3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

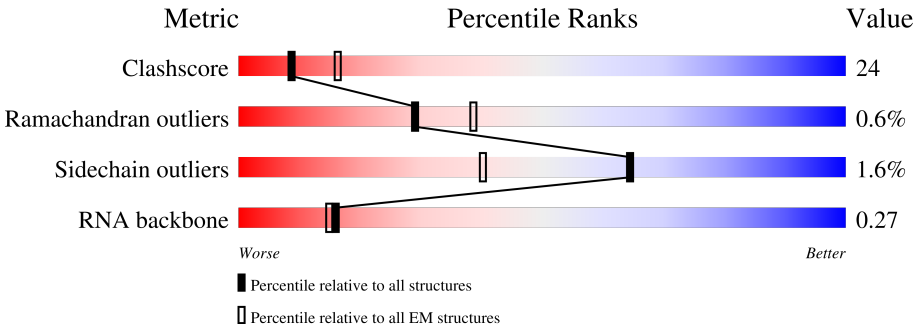
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	467	10% 53% 25% • 21%
2	B	436	17% 64% 35% •
3	C	262	14% 49% 32% 19%
4	D	204	25% 42% 20% 37%
5	E	346	23% 58% 35% • 6%
6	F	171	25% 58% 40% ••
7	G	374	16% 59% 37% ••

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Mol	Chain	Length	Quality of chain
8	H	168	29% 52% 43%
9	I	305	24% 44% 39% 16%
10	J	144	22% 51% 44%
11	K	194	24% 57% 34% 8%
12	L	186	16% 62% 33%
13	M	279	17% 48% 43% 7%
14	N	252	17% 50% 24% 25%
15	O	476	36% 37% 26% 36%
16	P	185	23% 52% 37% 11%
17	Q	234	19% 56% 35% 7%
18	R	480	30% 60% 38%
19	S	409	6% 25% 12% 63%
20	T	83	11% 35% 31% 34%
21	U	118	30% 42% 30% 5% 22%
22	V	151	23% 50% 41% 7%
23	W	186	6% 18% 11% 71%
24	X	513	28% 58% 32% 9%
25	Y	292	35% 58% 29% 13%
26	Z	197	18% 44% 30% 24%
27	BA	167	28% 35% 44% 17%
28	UA	203	19% 81% 19%
29	BB	156	24% 40% 36% 22%
30	Aw	187	22% 98%
31	Bj	185	40% 89% 9%
32	An	331	24% 90% 5% 5%

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Mol	Chain	Length	Quality of chain
33	Al	346	14% 75% 24%
34	BI	266	12% 47% 23% 30%
35	Az	152	14% 88% 9%
36	At	183	15% 90% 10%
37	BC	147	26% 61% 33% 5%
38	Ab	262	14% 99%
39	Ai	479	21% 99%
40	Ap	240	30% 89% 11%
41	Au	186	14% 85% 9% 5%
42	Aa	195	36% 87% 9%
43	Ao	284	13% 95%
44	BM	457	61% 40% 44% 15%
45	Ar	205	15% 95% 5%
46	Aj	503	15% 67% 32%
47	BH	229	23% 59% 34% 7%
48	Am	340	13% 96%
49	Aq	341	25% 72% 24%
50	BE	118	16% 42% 28% 29%
51	Ak	323	32% 92% 7%
52	BP	254	20% 46% 30% 23%
53	Ad	237	27% 86% 13%
54	BF	109	33% 57% 36% 7%
55	Av	192	24% 81% 19%
56	Af	155	27% 88% 10%
57	As	249	12% 39% 61%

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Mol	Chain	Length	Quality of chain
58	Ae	311	15% 92% 6%
59	Ac	291	33% 91% 8%
60	Ah	570	26% 78% 21%
61	BD	102	17% 55% 39% 5%
62	Ay	174	18% 78% 18%
63	Ag	244	20% 93% 5%
64	Ax	216	11% 72% 6% 23%
65	BL	380	12% 39% 39% 19%
66	BO	190	26% 28% 48% 5% 18%
67	BG	1347	94%
68	UB	67	16% 84% 16%
69	UC	144	72% 88% 10%
70	UD	95	33% 89% 11%
71	1	9070	5% 5% 88%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
72	ZN	BG	1401	-	-	X	-
72	ZN	T	101	-	-	X	-

2 Entry composition

There are 73 unique types of molecules in this entry. The entry contains 143667 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	368	2996	1929	496	556	15	0	0

- Molecule 2 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	435	3513	2237	615	642	19	0	0

- Molecule 3 is a protein called RIBOSOMAL_L9 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	212	1772	1144	303	321	4	0	0

- Molecule 4 is a protein called uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	128	1036	656	198	177	5	0	0

- Molecule 5 is a protein called Putative ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	326	2668	1704	480	470	14	0	0

- Molecule 6 is a protein called 50S ribosomal protein L13-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	170	1435	919	261	243	12	0	0

- Molecule 7 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	365	Total	C	N	O	S	0	0
			3012	1917	555	531	9		

- Molecule 8 is a protein called Ribosomal_L16 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	162	Total	C	N	O	S	0	0
			1305	836	239	226	4		

- Molecule 9 is a protein called Putative 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	257	Total	C	N	O	S	0	0
			2153	1362	406	372	13		

- Molecule 10 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	141	Total	C	N	O	S	0	0
			1146	727	211	202	6		

- Molecule 11 is a protein called bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	179	Total	C	N	O	S	0	0
			1467	910	289	258	10		

- Molecule 12 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	178	Total	C	N	O	S	0	0
			1419	907	257	250	5		

- Molecule 13 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	259	Total	C	N	O	S	0	0
			2116	1345	385	371	15		

- Molecule 14 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	189	Total	C	N	O	S	0	0
			1599	1031	296	269	3		

- Molecule 15 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	307	Total	C	N	O	S	0	0
			2537	1600	455	475	7		

- Molecule 16 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	165	Total	C	N	O	S	0	0
			1367	856	266	238	7		

- Molecule 17 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	217	Total	C	N	O	S	0	0
			1785	1127	331	316	11		

- Molecule 18 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	472	Total	C	N	O	S	0	0
			3755	2377	662	704	12		

- Molecule 19 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	150	Total	C	N	O	S	0	0
			1244	782	247	207	8		

- Molecule 20 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	55	Total	C	N	O	S	0	0
			487	311	93	78	5		

- Molecule 21 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	92	Total	C	N	O	S	0	0
			744	472	142	125	5		

- Molecule 22 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	141	Total	C	N	O	S	0	0
			1202	755	242	197	8		

- Molecule 23 is a protein called bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	54	Total	C	N	O	S	0	0
			465	299	89	74	3		

- Molecule 24 is a protein called mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	468	Total	C	N	O	S	0	0
			3733	2365	657	694	17		

- Molecule 25 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	255	Total	C	N	O	S	0	0
			2067	1287	373	402	5		

- Molecule 26 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	150	Total	C	N	O	S	0	0
			1223	784	224	211	4		

- Molecule 27 is a protein called mL94.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BA	138	Total	C	N	O	S	0	0
			1038	648	188	197	5		

- Molecule 28 is a protein called UA.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	UA	203	Total	C	N	O	0	0
			1015	609	203	203		

- Molecule 29 is a protein called mL95.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	BB	122	Total	C	N	O	0	0
			1028	663	189	176		

- Molecule 30 is a protein called mL89.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Aw	185	Total	C	N	O	S	0	0
			1509	949	289	268	3		

- Molecule 31 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bj	168	Total	C	N	O	S	0	0
			1358	865	255	231	7		

- Molecule 32 is a protein called mL76.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	An	314	Total	C	N	O	S	0	0
			2605	1643	487	470	5		

- Molecule 33 is a protein called mL74.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Al	264	Total	C	N	O	S	0	0
			2152	1371	374	399	8		

- Molecule 34 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BI	186	Total	C	N	O	S	0	0
			1409	895	242	264	8		

- Molecule 35 is a protein called mL93.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Az	138	Total	C	N	O	S	0	0
			1215	782	216	211	6		

- Molecule 36 is a protein called mL86.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	At	165	Total	C	N	O	S	0	0
			1346	824	260	254	8		

- Molecule 37 is a protein called mL96.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	140	Total	C	N	O	S	0	0
			1114	693	205	207	9		

- Molecule 38 is a protein called L51_S25_CI-B8 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ab	260	Total	C	N	O	S	0	0
			2185	1365	416	397	7		

- Molecule 39 is a protein called mL69.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ai	476	Total	C	N	O	S	0	0
			3789	2419	654	694	22		

- Molecule 40 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ap	214	Total	C	N	O	S	0	0
			1775	1111	327	328	9		

- Molecule 41 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Au	176	Total	C	N	O	S	0	0
			1490	945	292	245	8		

- Molecule 42 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Aa	178	Total	C	N	O	S	0	0
			1417	884	270	256	7		

- Molecule 43 is a protein called mL79.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ao	275	Total	C	N	O	S	0	0
			2276	1433	429	402	12		

- Molecule 44 is a protein called mL70.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BM	389	Total	C	N	O	S	0	0
			3069	1954	548	551	16		

- Molecule 45 is a protein called mL84.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ar	195	Total	C	N	O	S	0	0
			1644	1054	295	288	7		

- Molecule 46 is a protein called mL72.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Aj	341	Total	C	N	O	S	0	0
			2766	1756	508	491	11		

- Molecule 47 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BH	214	Total	C	N	O	S	0	0
			1659	1050	290	310	9		

- Molecule 48 is a protein called mL75.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Am	330	Total	C	N	O	S	0	0
			2708	1727	491	474	16		

- Molecule 49 is a protein called mL82.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Aq	258	Total	C	N	O	S	0	0
			2074	1296	406	360	12		

- Molecule 50 is a protein called mL98.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	BE	84	Total	C	N	O	0	0
			700	447	125	128		

- Molecule 51 is a protein called mL73.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ak	300	Total	C	N	O	S	0	0
			2352	1489	421	429	13		

- Molecule 52 is a protein called mL52,mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BP	195	Total	C	N	O	S	0	0
			1593	1014	288	288	3		

- Molecule 53 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Ad	207	Total	C	N	O	S	0	0
			1632	1049	289	286	8		

- Molecule 54 is a protein called mL99.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BF	101	Total	C	N	O	S	0	0
			851	530	165	154	2		

- Molecule 55 is a protein called mL88.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Av	155	Total	C	N	O	S	0	0
			1300	828	230	234	8		

- Molecule 56 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Af	139	Total	C	N	O	S	0	0
			1132	709	215	207	1		

- Molecule 57 is a protein called mL85.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	As	97	Total	C	N	O	S	0	0
			787	495	139	148	5		

- Molecule 58 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Ae	291	Total	C	N	O	S	0	0
			2359	1526	418	404	11		

- Molecule 59 is a protein called MRP-L46 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Ac	268	Total	C	N	O	S	0	0
			2174	1375	389	405	5		

- Molecule 60 is a protein called mL68.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Ah	452	Total	C	N	O	S	0	0
			3686	2338	651	679	18		

- Molecule 61 is a protein called mL97.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BD	97	Total	C	N	O	S	0	0
			807	499	160	140	8		

- Molecule 62 is a protein called C2H2-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Ay	142	Total	C	N	O	S	0	0
			1226	774	228	217	7		

- Molecule 63 is a protein called mL54/69.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Ag	231	Total	C	N	O	S	0	0
			1916	1211	356	340	9		

- Molecule 64 is a protein called LIM zinc-binding domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Ax	167	Total	C	N	O	S	0	0
			1388	876	268	233	11		

- Molecule 65 is a protein called Putative ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BL	309	Total	C	N	O	S	0	0
			2497	1594	464	427	12		

- Molecule 66 is a protein called Putative ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BO	155	Total	C	N	O	S	0	0
			1239	772	253	205	9		

- Molecule 67 is a protein called mL100.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BG	85	Total	C	N	O	S	0	0
			643	400	122	115	6		

- Molecule 68 is a protein called UB.

Mol	Chain	Residues	Atoms				AltConf	Trace
68	UB	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 69 is a protein called UC.

Mol	Chain	Residues	Atoms				AltConf	Trace
69	UC	144	Total	C	N	O	0	0
			720	432	144	144		

- Molecule 70 is a protein called UD.

Mol	Chain	Residues	Atoms				AltConf	Trace
70	UD	95	Total 475	C 285	N 95	O 95	0	0

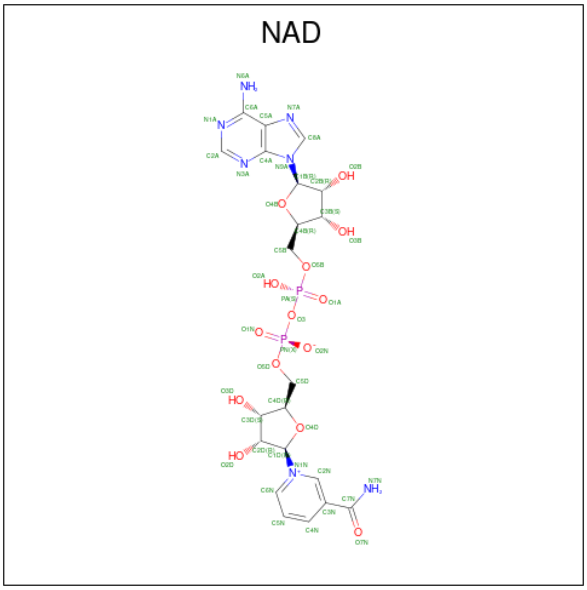
- Molecule 71 is a RNA chain called Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	1	1087	Total 22918	C 10319	N 3839	O 7673	P 1087	0	0

- Molecule 72 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
72	T	1	Total 1	Zn 1	0
72	W	1	Total 1	Zn 1	0
72	BD	1	Total 1	Zn 1	0
72	Ax	2	Total 2	Zn 2	0
72	BG	1	Total 1	Zn 1	0

- Molecule 73 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

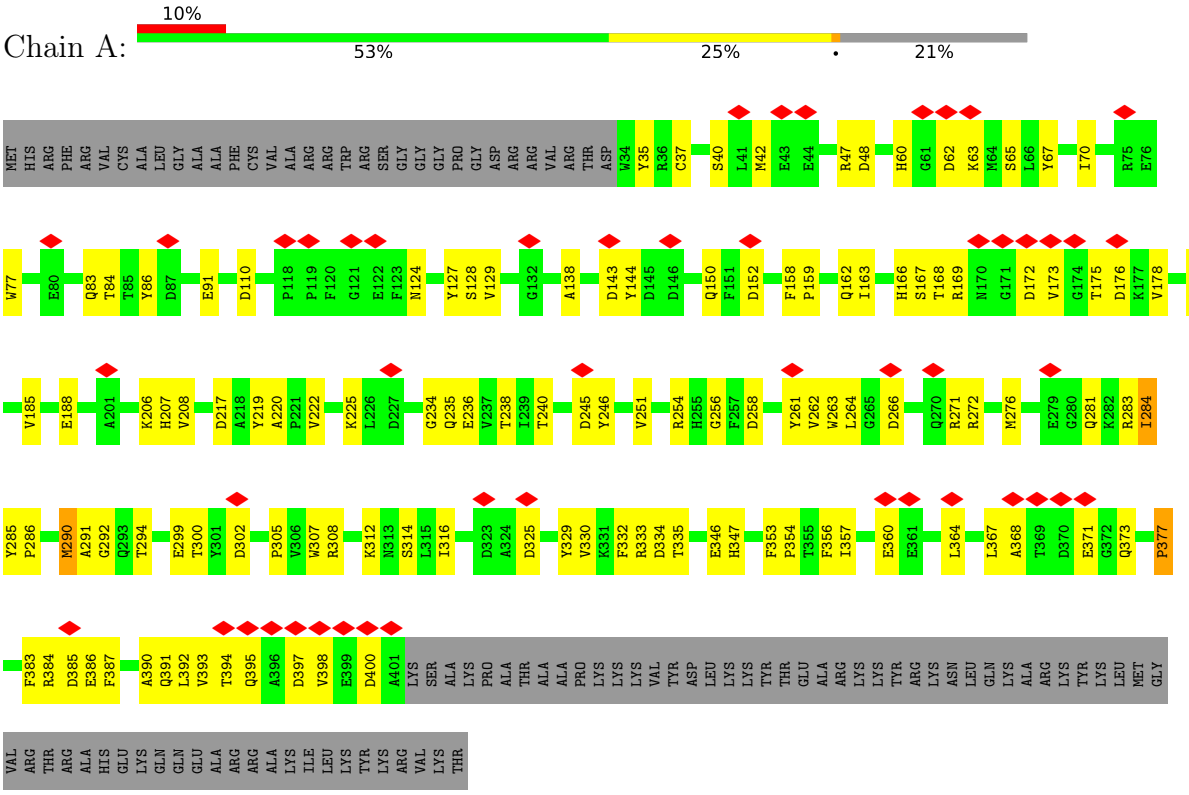


Mol	Chain	Residues	Atoms					AltConf
73	Ag	1	Total	C	N	O	P	0
			44	21	7	14	2	

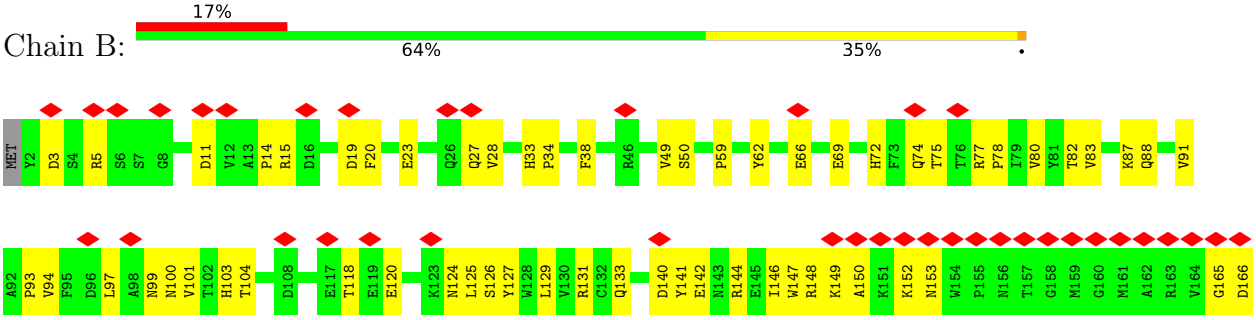
3 Residue-property plots (i)

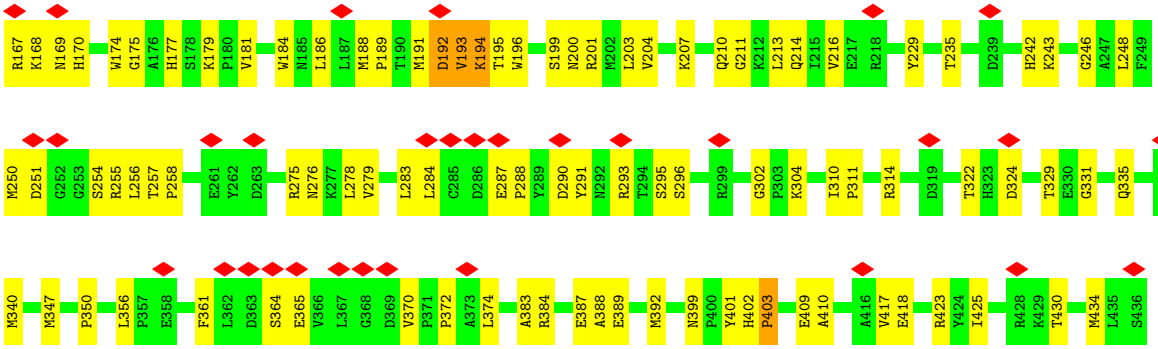
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ribosomal protein L3-like protein



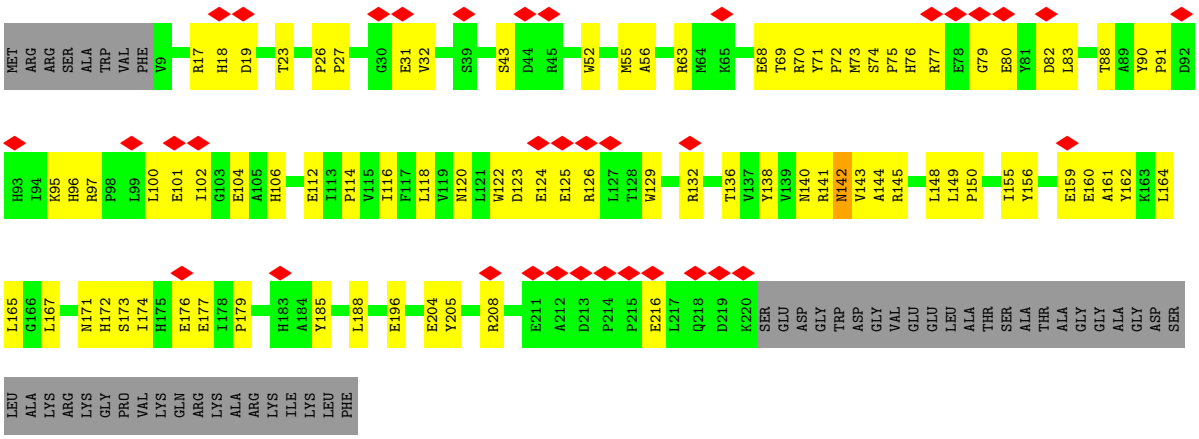
• Molecule 2: uL4m





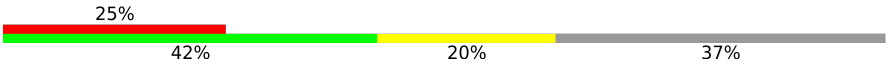
• Molecule 3: RIBOSOMAL_L9 domain-containing protein

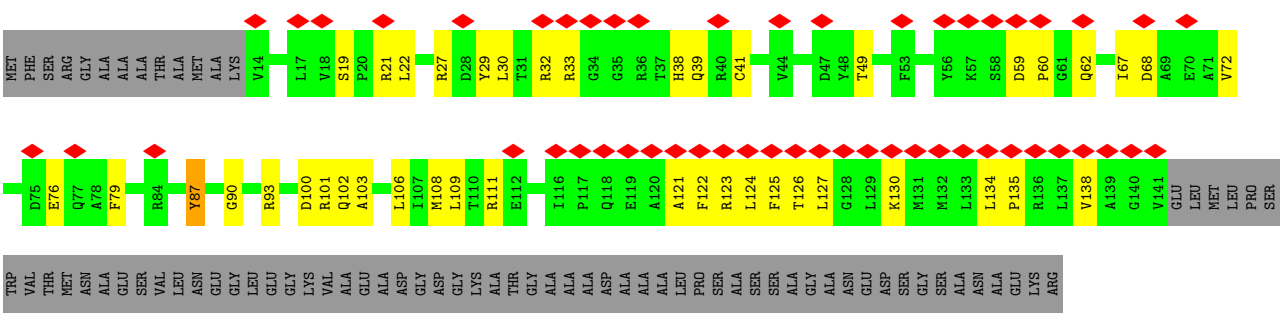
Chain C:



• Molecule 4: uL10m

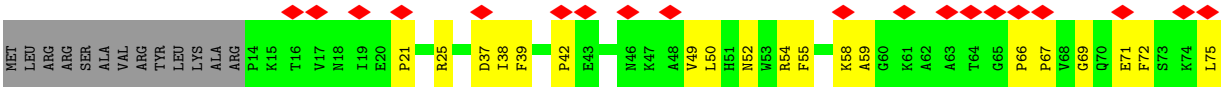
Chain D:

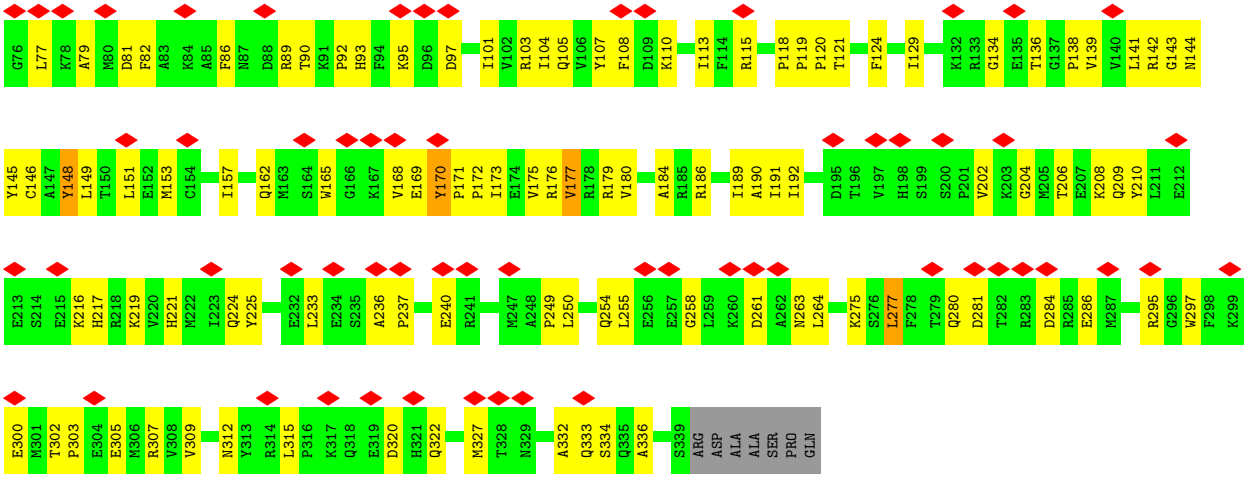




• Molecule 5: Putative ribosomal protein L11

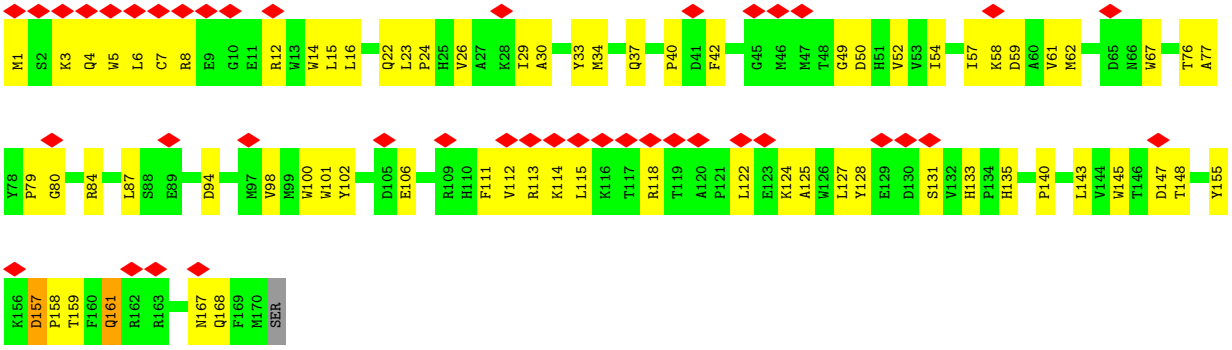
Chain E:





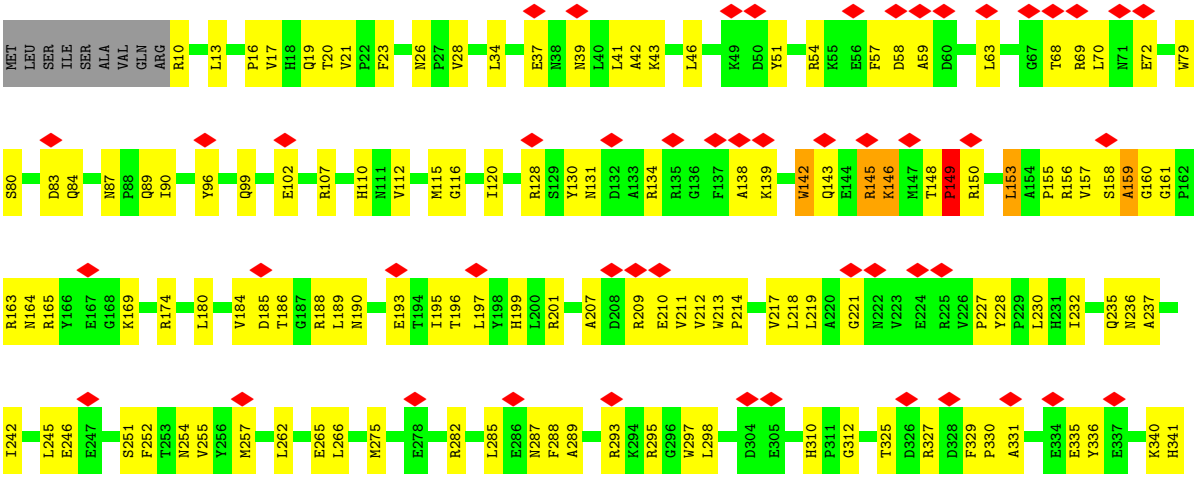
• Molecule 6: 50S ribosomal protein L13-like protein

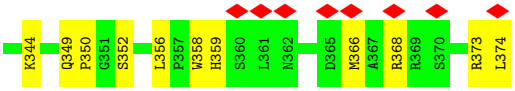
Chain F:



• Molecule 7: Ribosomal_L18e/L15P domain-containing protein

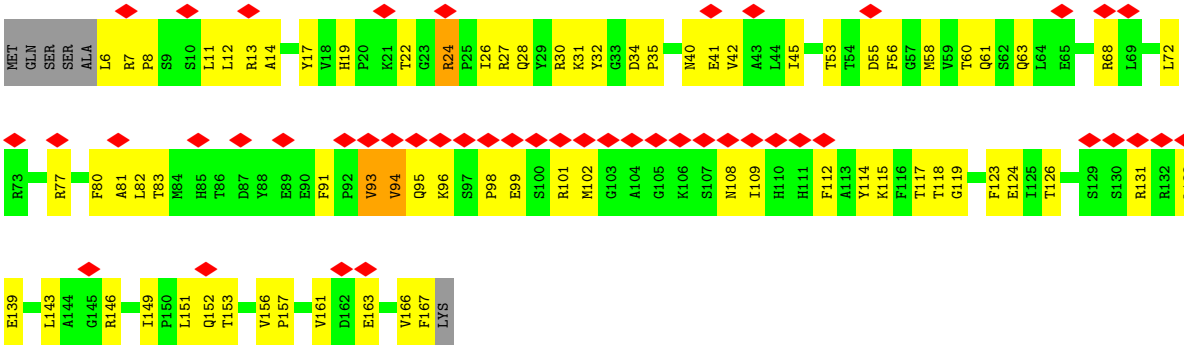
Chain G:





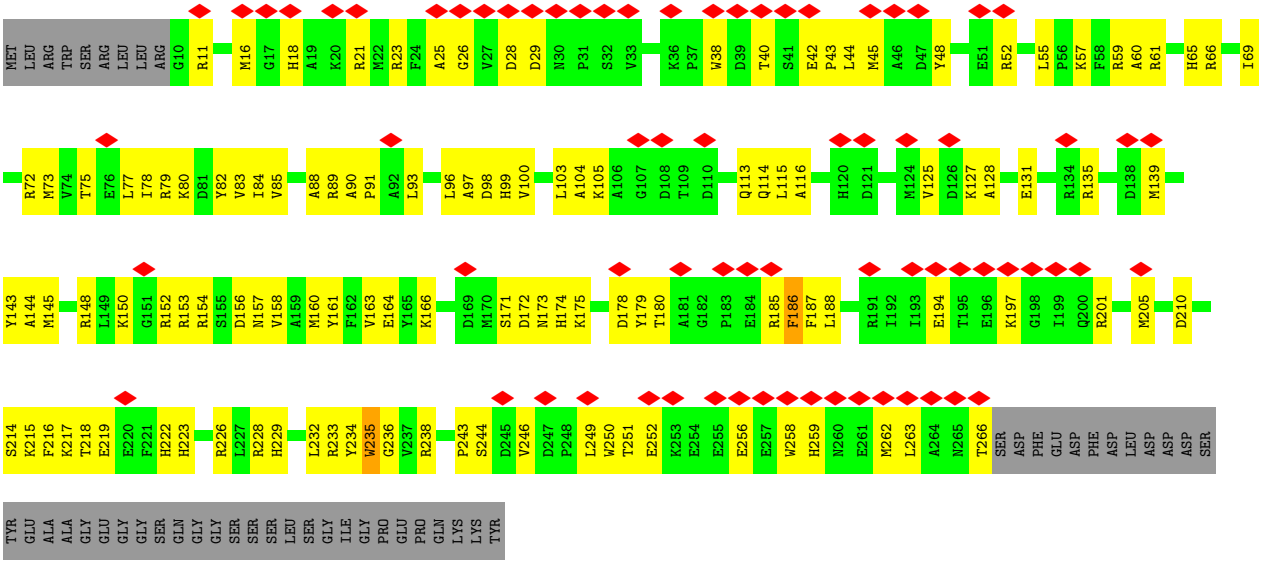
• Molecule 8: Ribosomal_L16 domain-containing protein

Chain H:



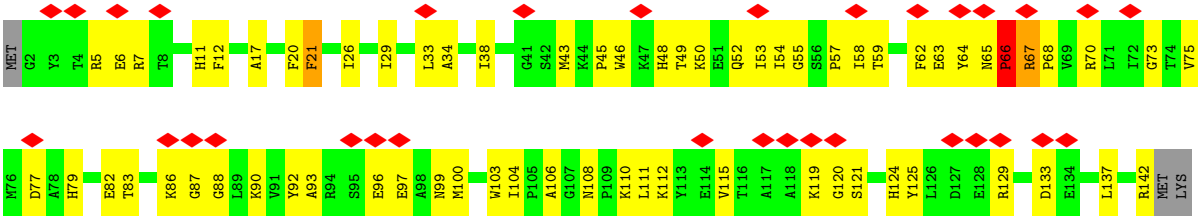
• Molecule 9: Putative 50S ribosomal protein L17

Chain I:



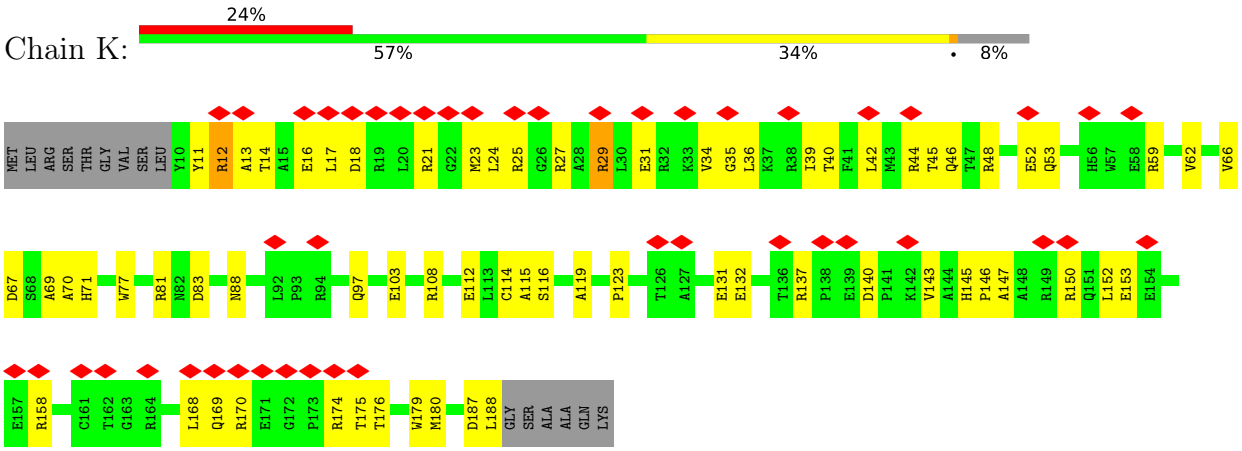
• Molecule 10: bL19m

Chain J:



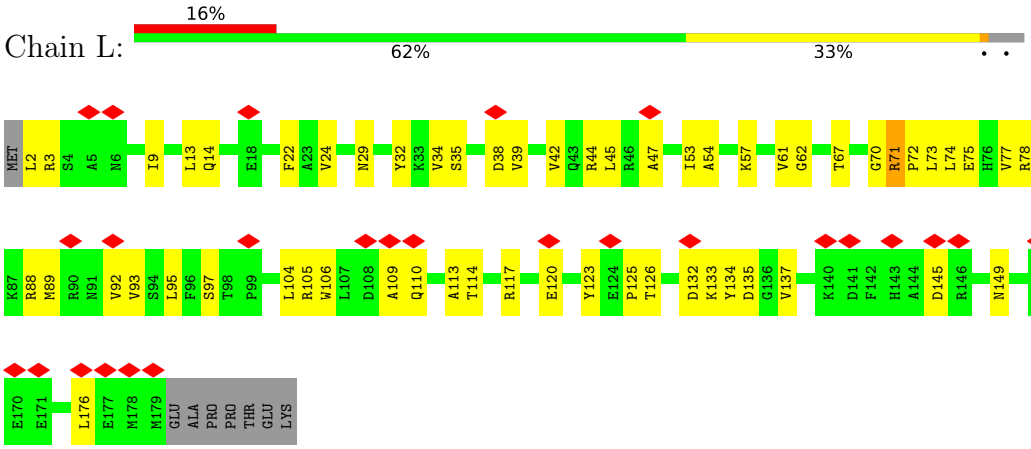
• Molecule 11: bL20

Chain K:



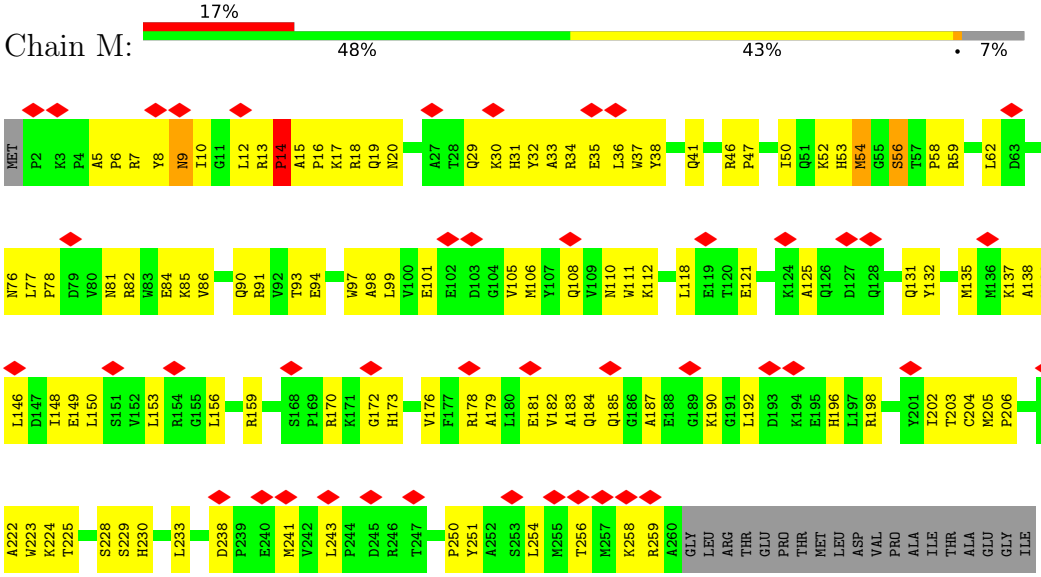
• Molecule 12: bL21m

Chain L:



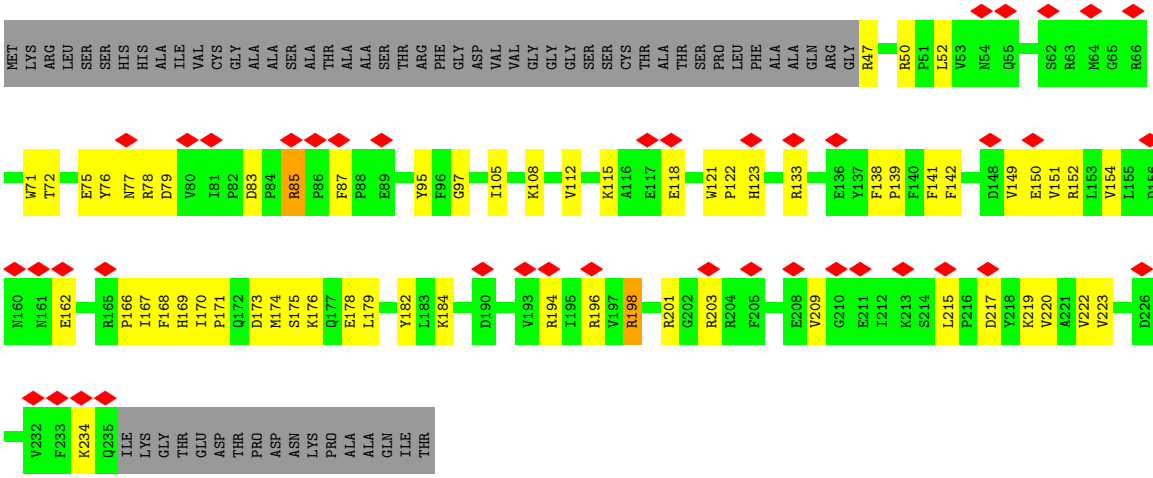
• Molecule 13: uL22m

Chain M:



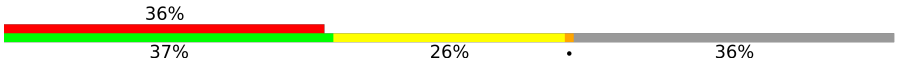
• Molecule 14: uL23m

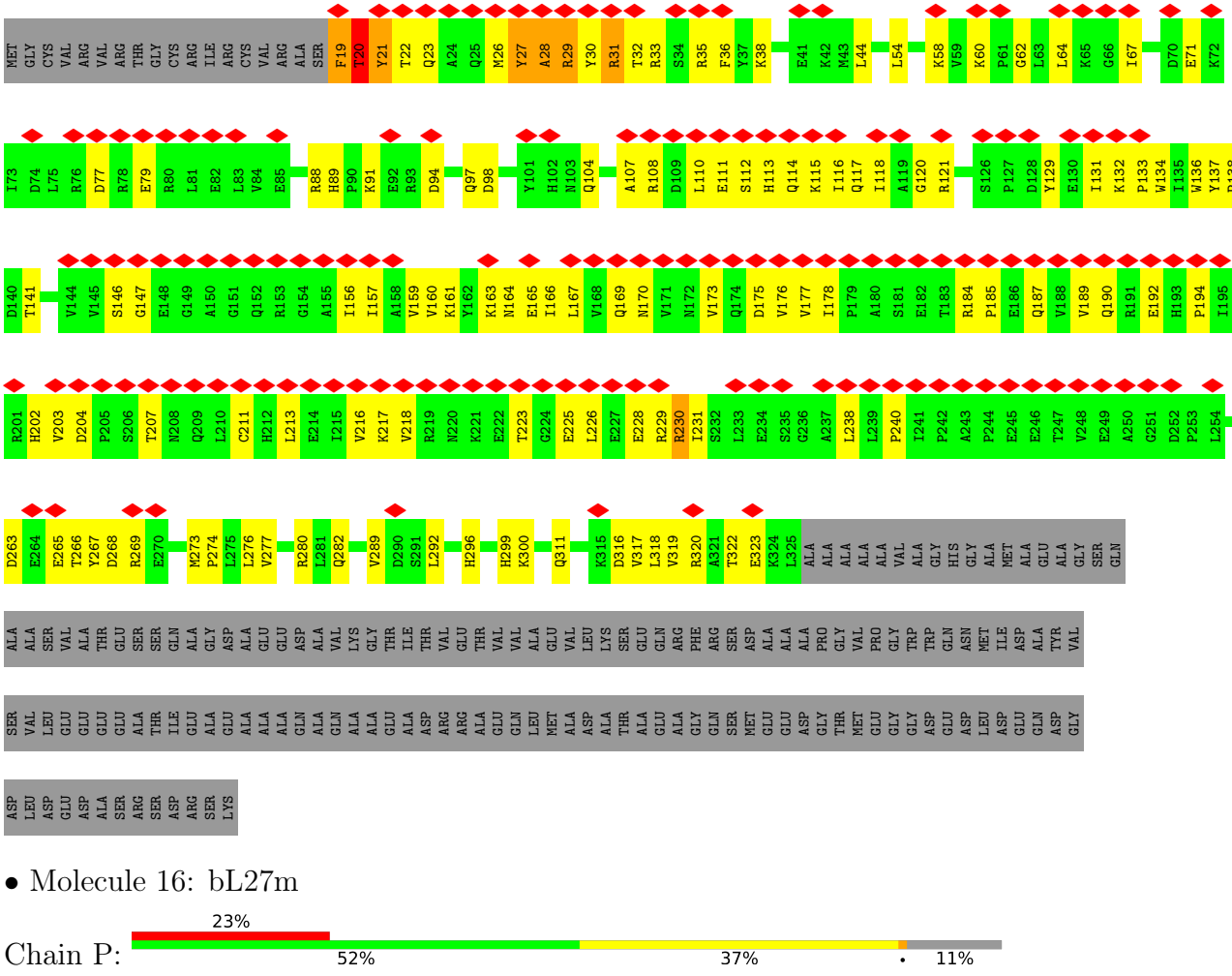
Chain N:



• Molecule 15: uL24m

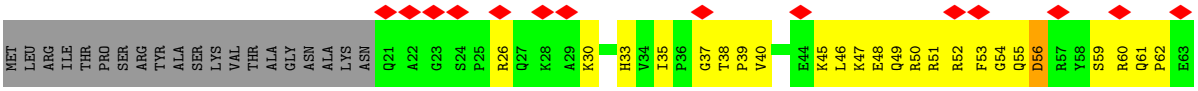
Chain O:

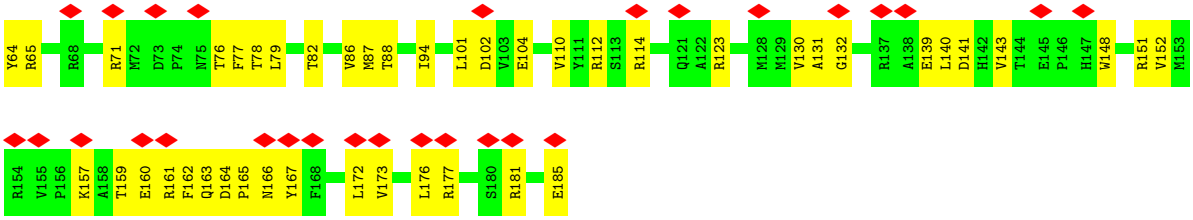




• Molecule 16: bL27m

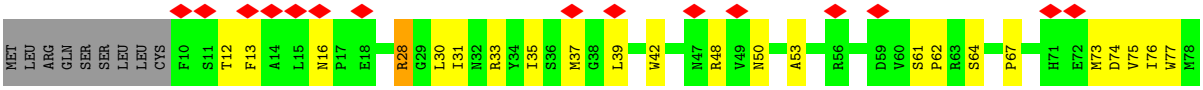
Chain P:

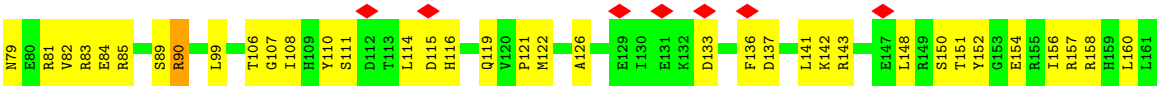


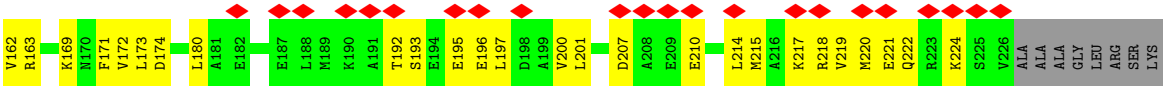


• Molecule 17: bL28m

Chain Q:

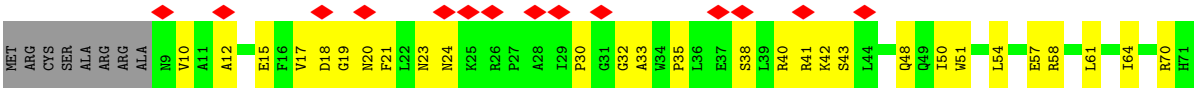


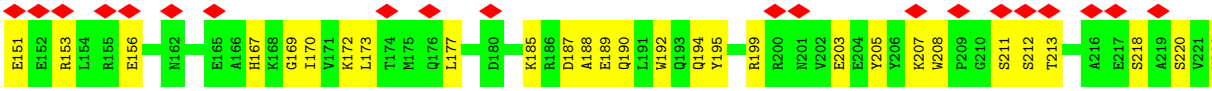


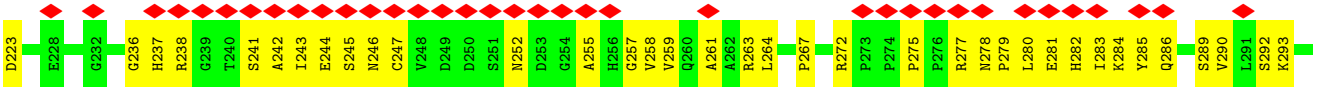


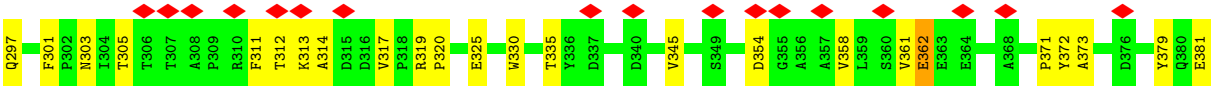
• Molecule 18: uL29m

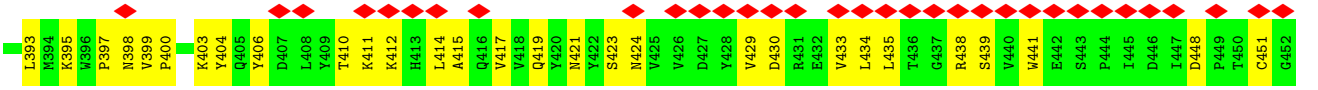
Chain R:

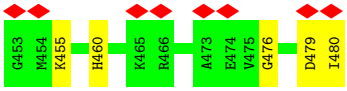






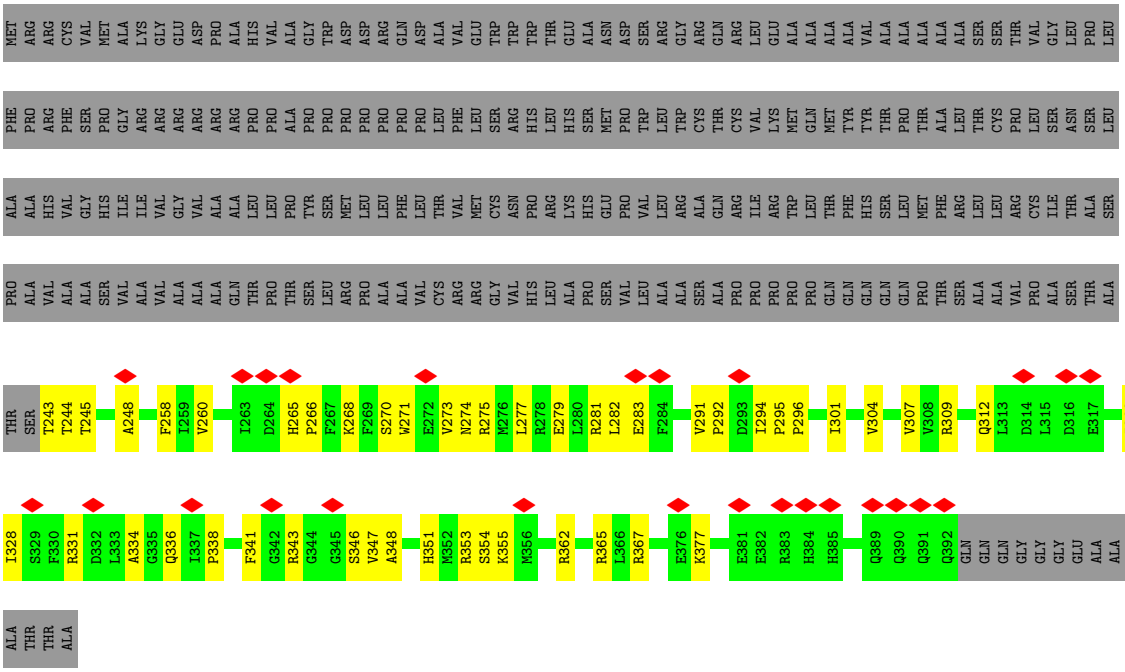






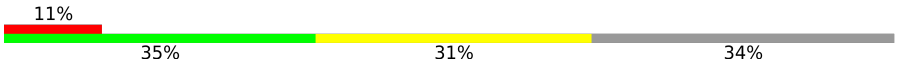
• Molecule 19: uL30m

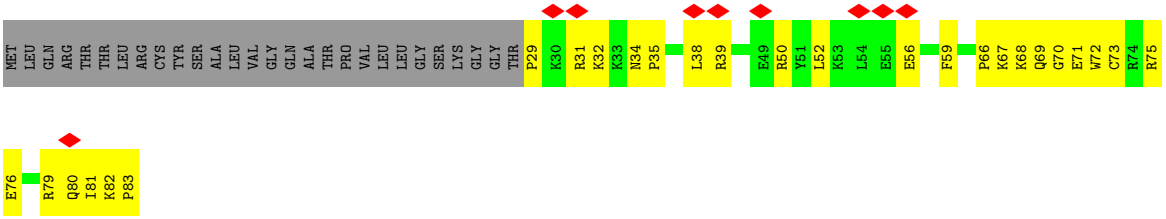
Chain S:



• Molecule 20: bL32m

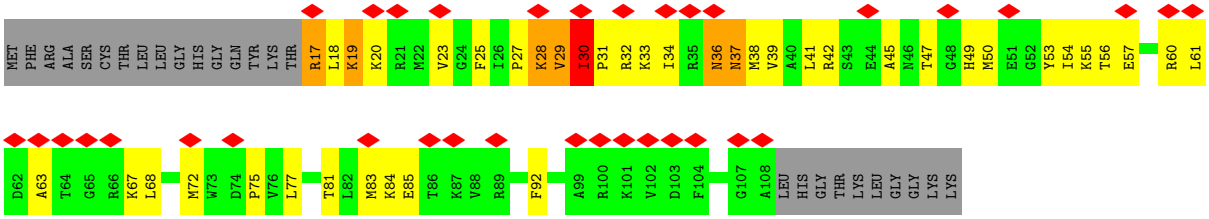
Chain T:





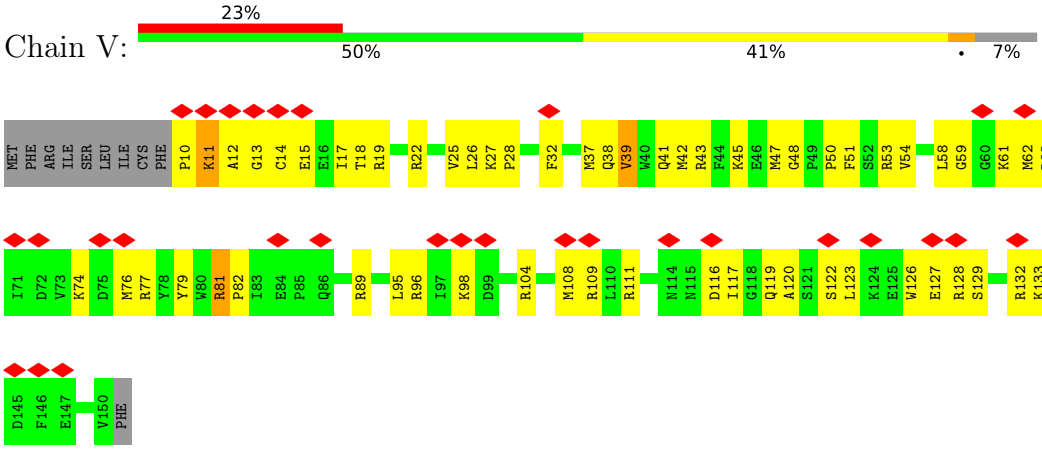
• Molecule 21: bL33m

Chain U:



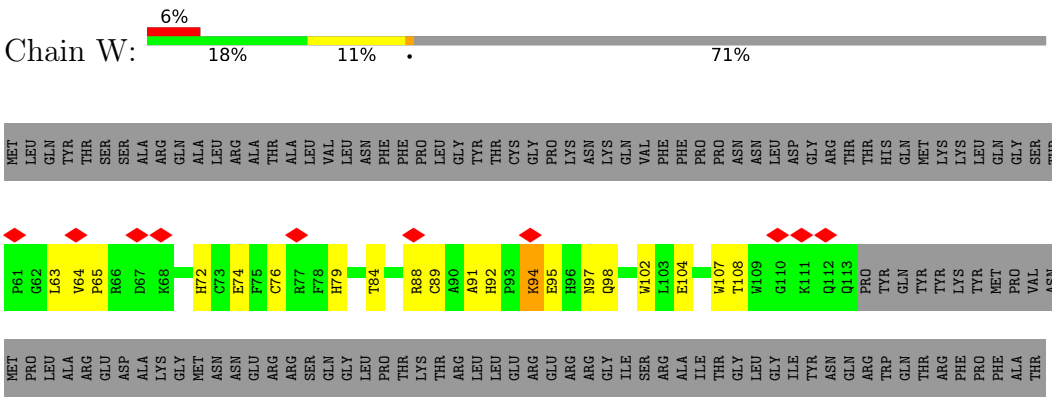
• Molecule 22: bL35m

Chain V:



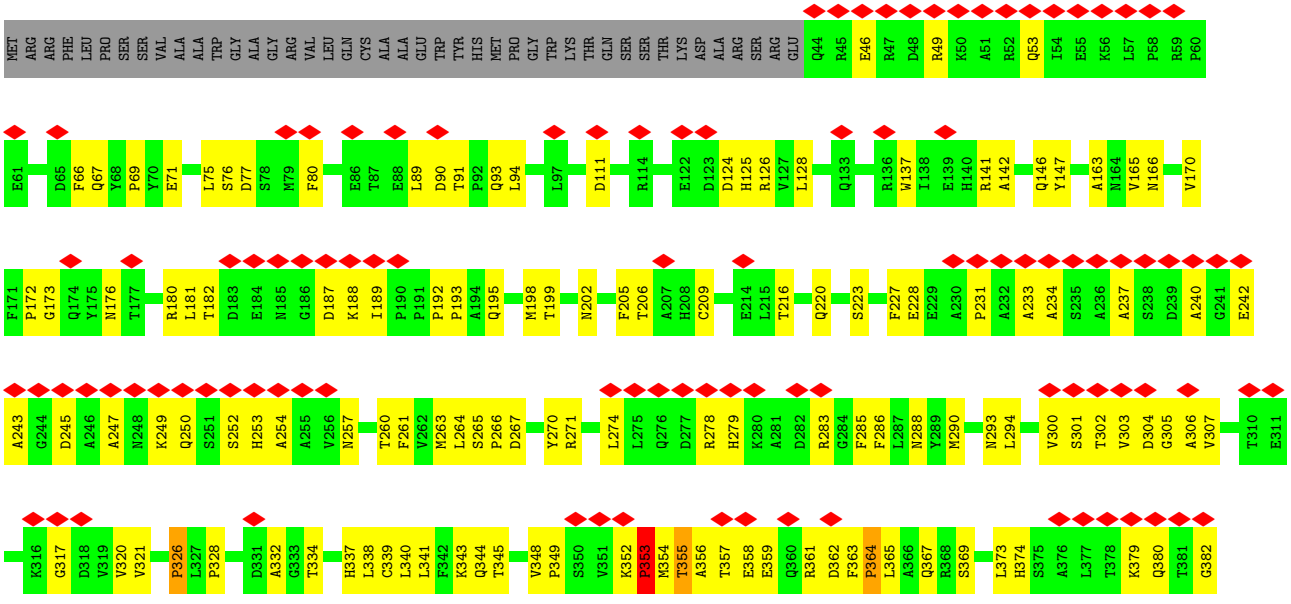
• Molecule 23: bL36m

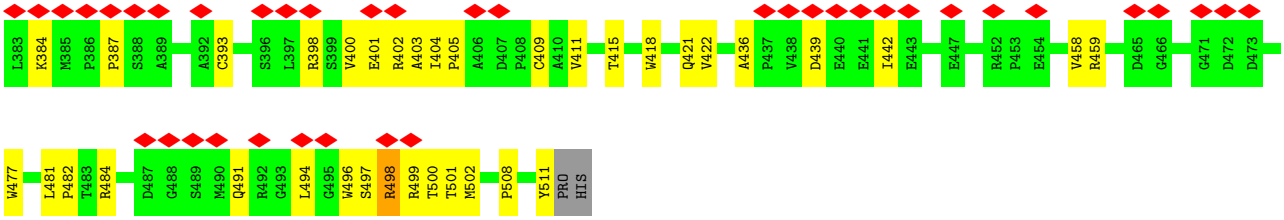
Chain W:



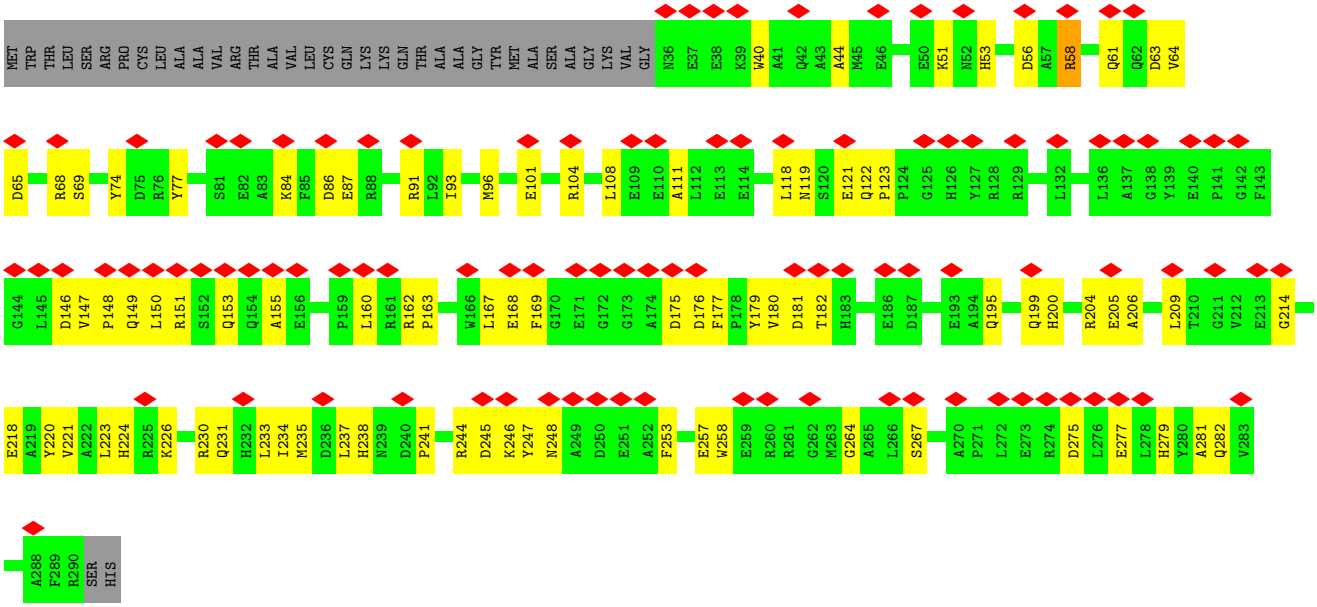
• Molecule 24: mL38

Chain X:

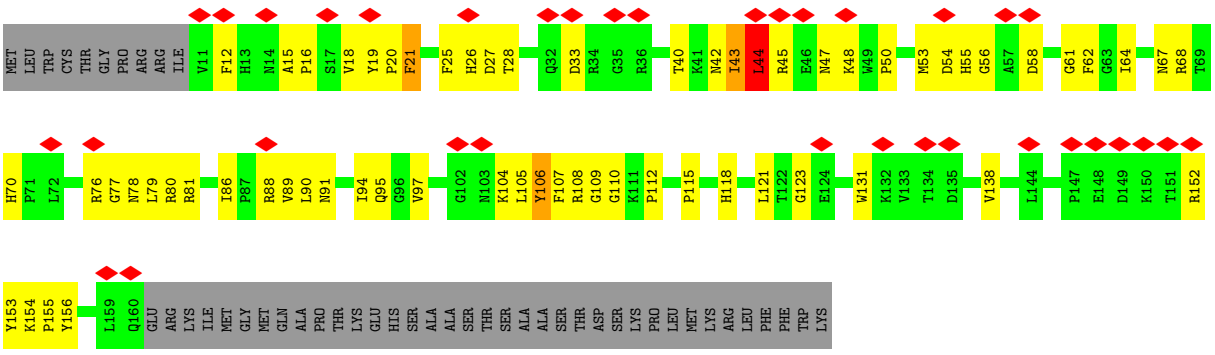




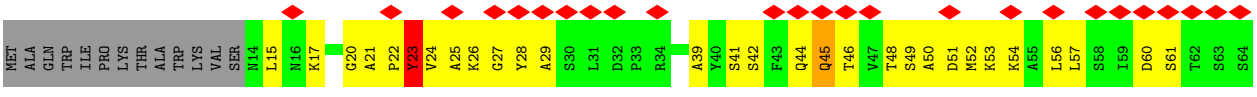
• Molecule 25: mL40

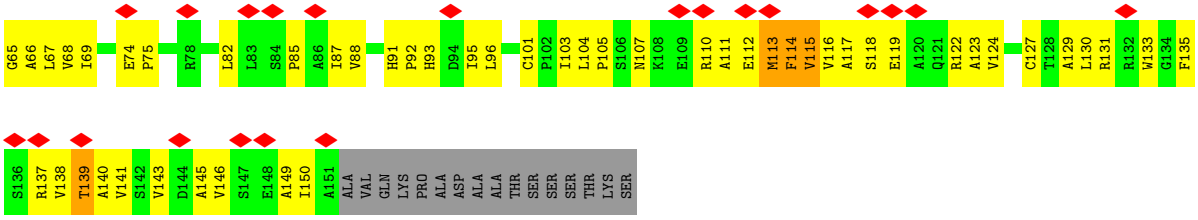


• Molecule 26: mL41

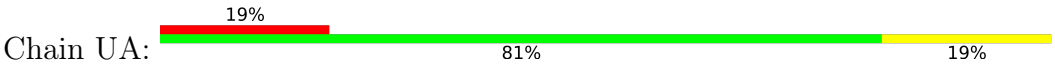


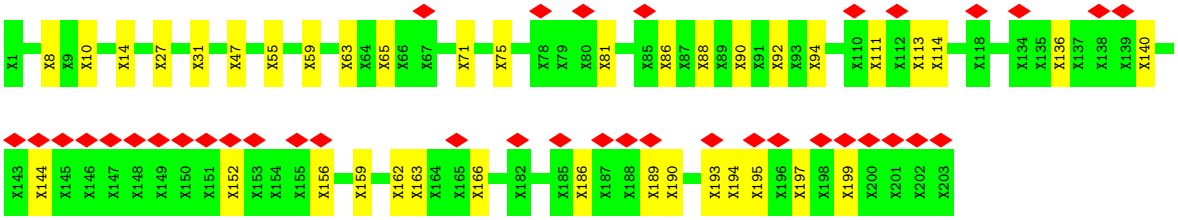
• Molecule 27: mL94



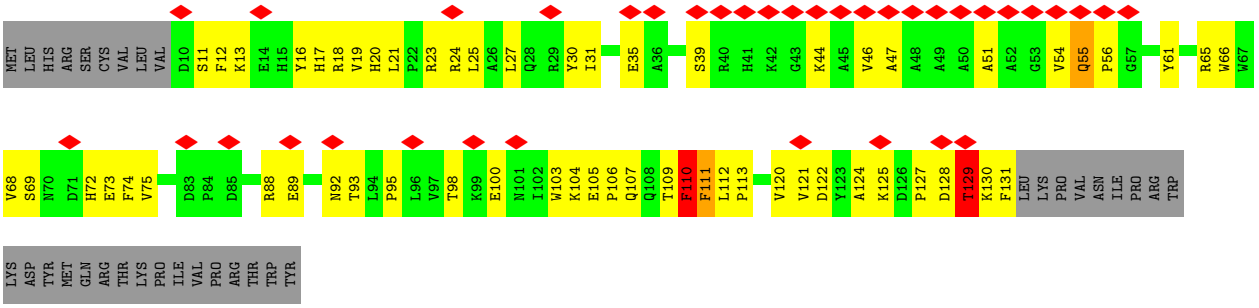


• Molecule 28: UA

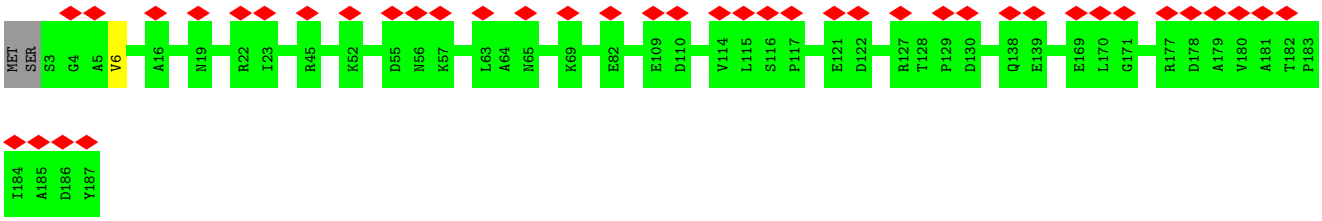




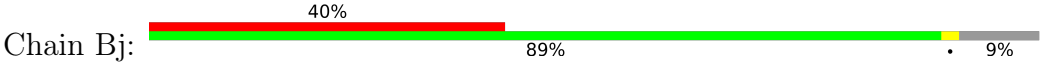
• Molecule 29: mL95

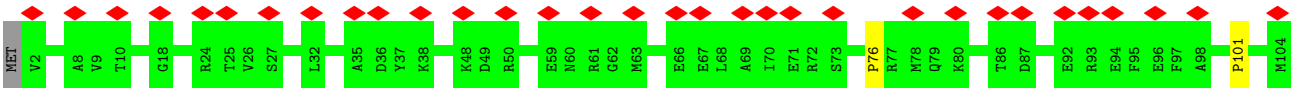


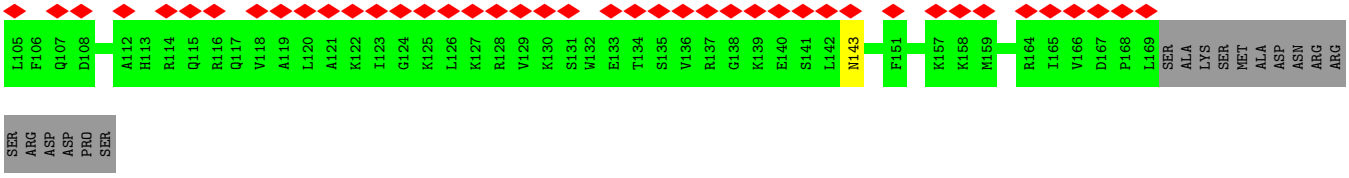
• Molecule 30: mL89



• Molecule 31: bL31m

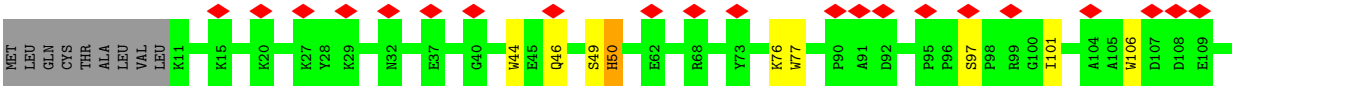


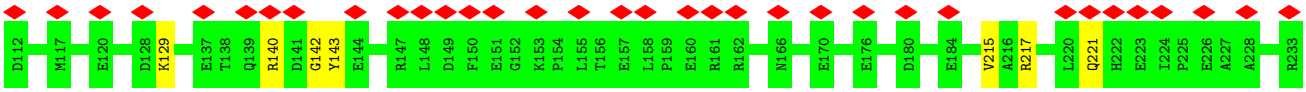


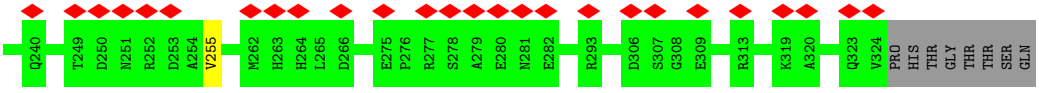


• Molecule 32: mL76

Chain An:

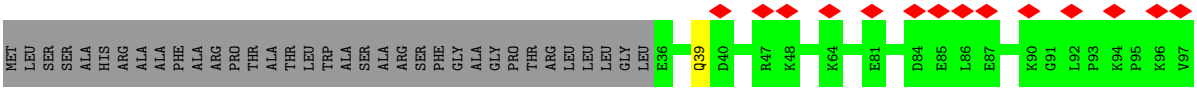


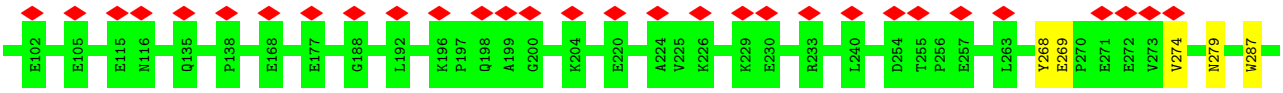


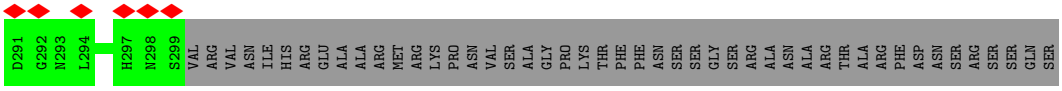


• Molecule 33: mL74

Chain Al:

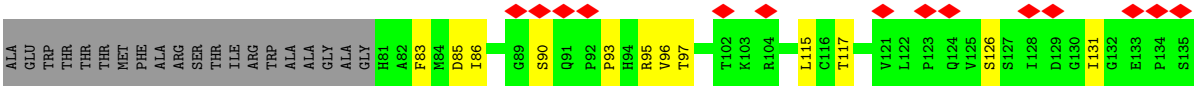


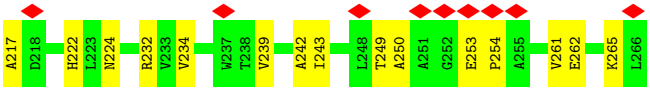




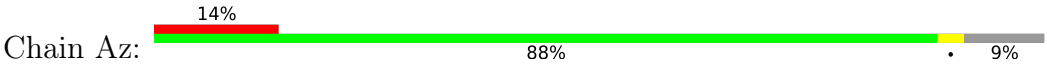
• Molecule 34: Peptidyl-prolyl cis-trans isomerase

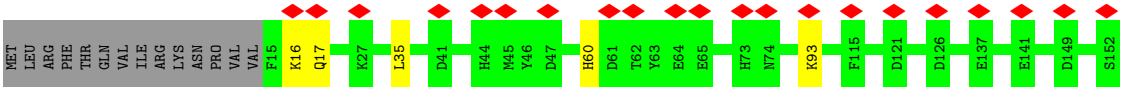
Chain BI:



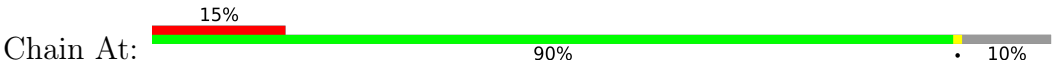


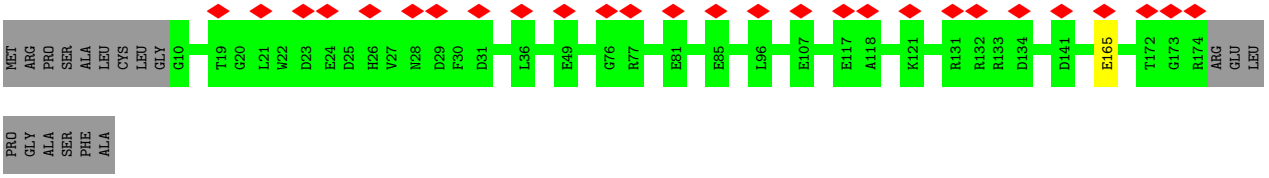
• Molecule 35: mL93



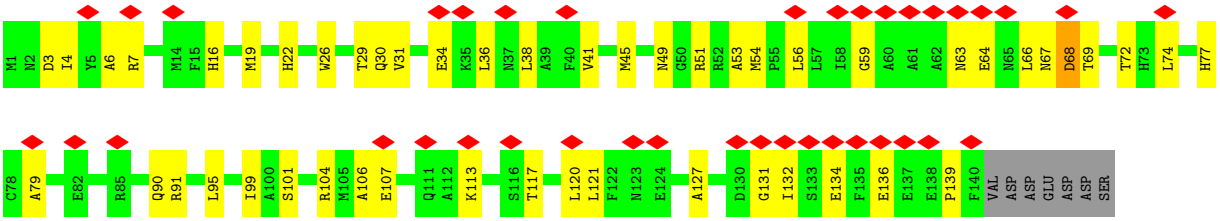


• Molecule 36: mL86

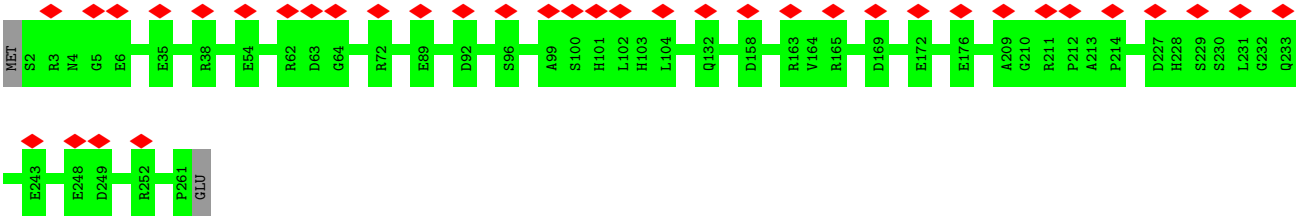




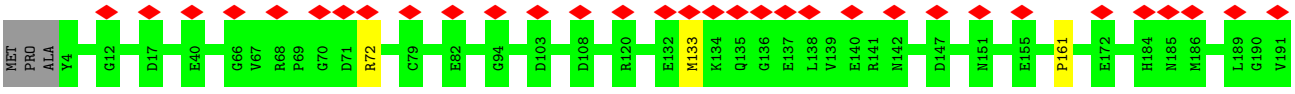
• Molecule 37: mL96

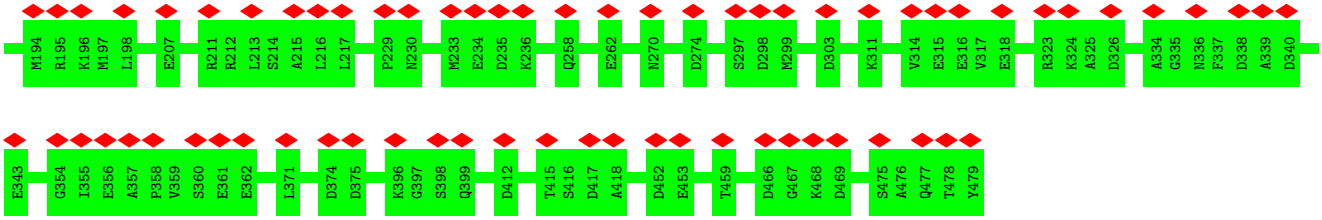


• Molecule 38: L51_S25_CI-B8 domain-containing protein

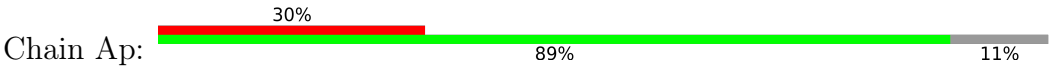


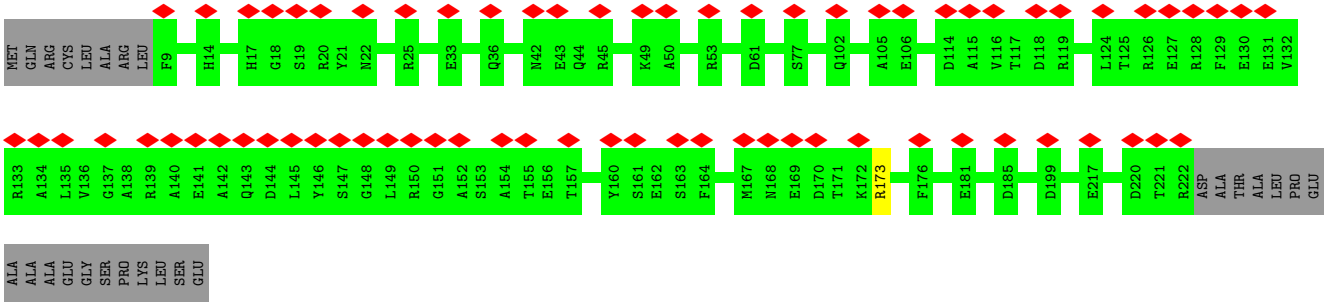
• Molecule 39: mL69



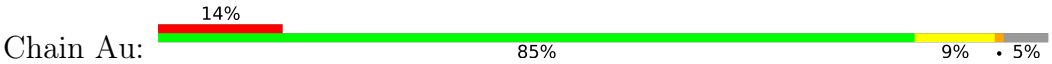


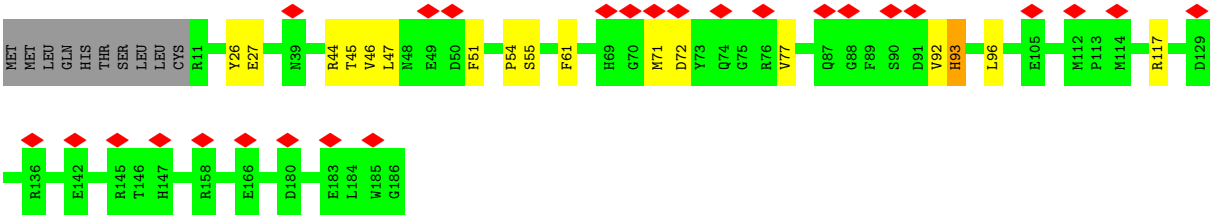
• Molecule 40: mL80



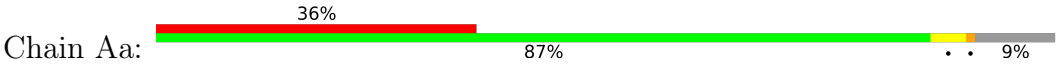


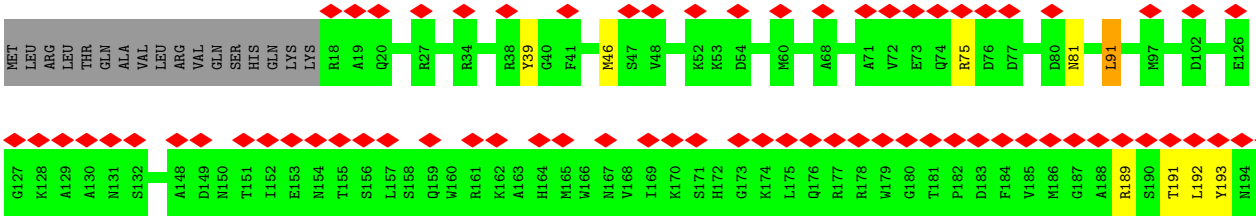
• Molecule 41: mL87



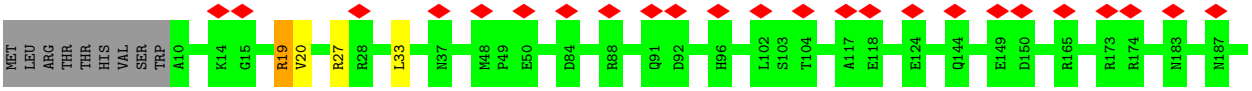


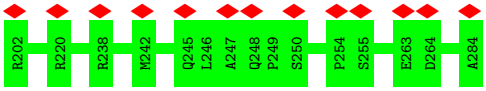
• Molecule 42: mL42





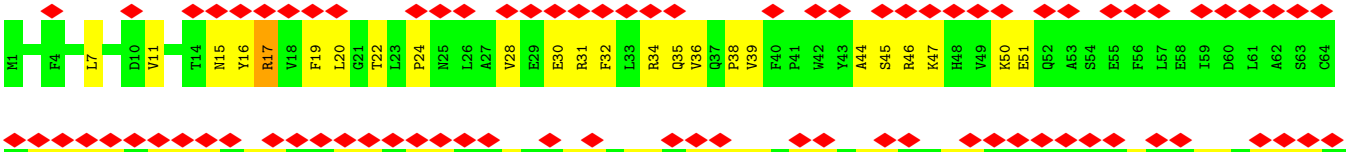
• Molecule 43: mL79

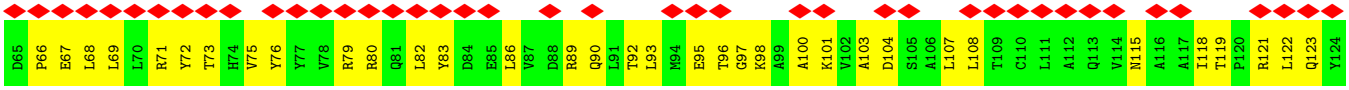


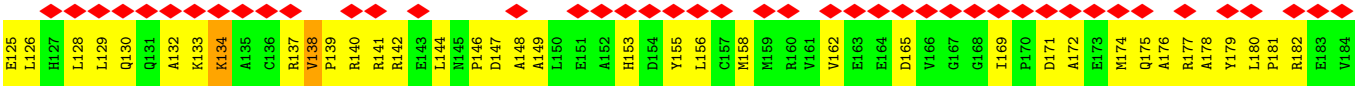


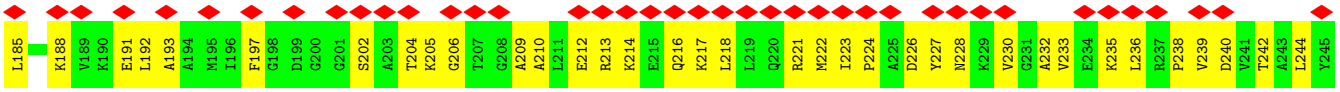
• Molecule 44: mL70

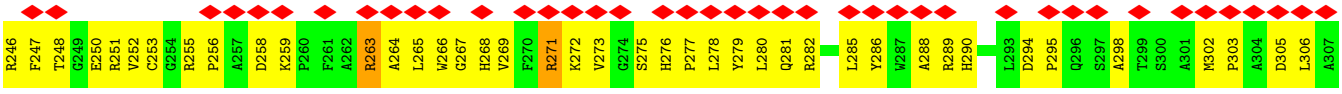
Chain BM:

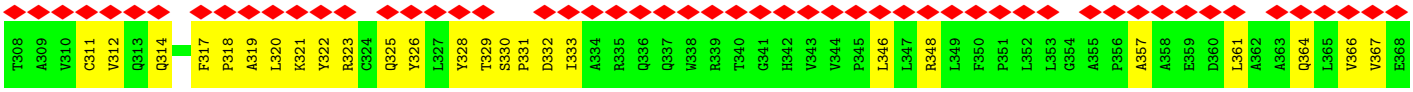


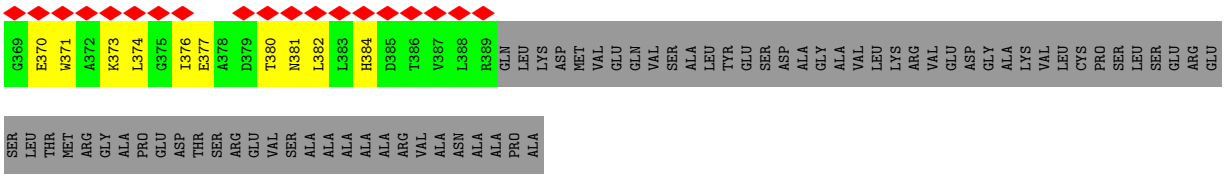






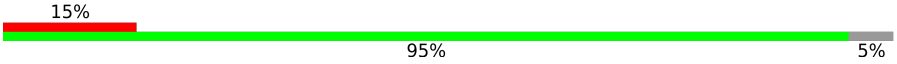


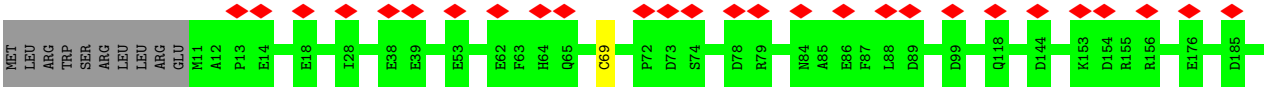


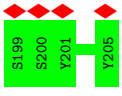


• Molecule 45: mL84

Chain Ar:

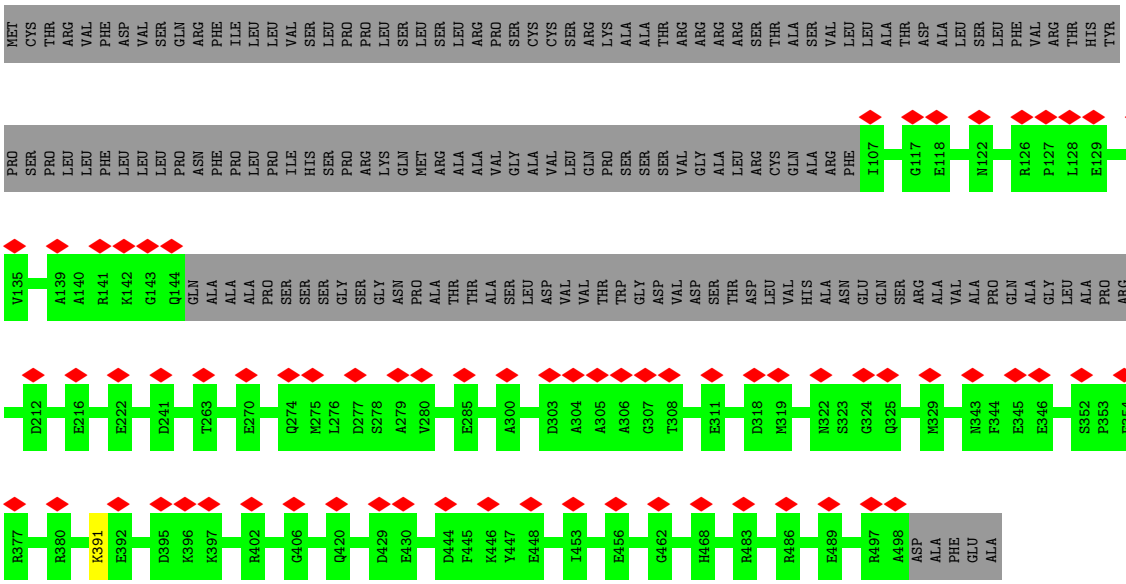






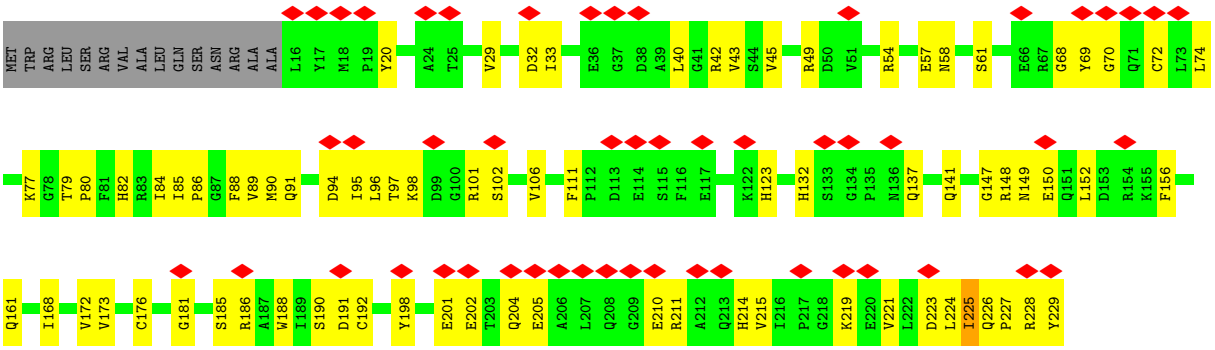
• Molecule 46: mL72

Chain Aj:



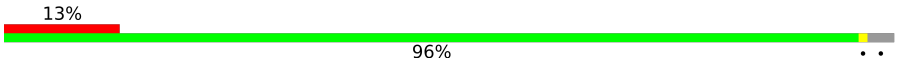
• Molecule 47: Peptidyl-prolyl cis-trans isomerase

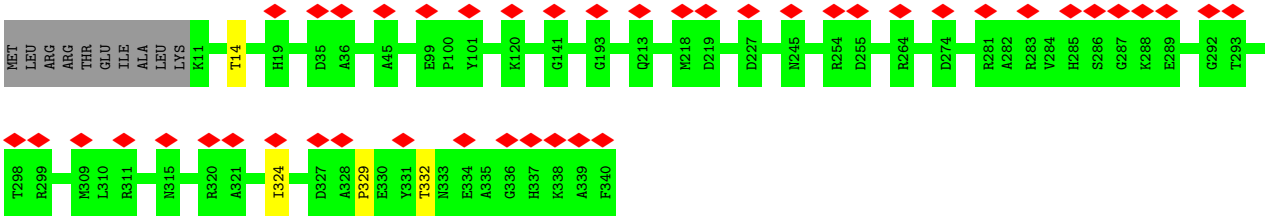
Chain BH:



• Molecule 48: mL75

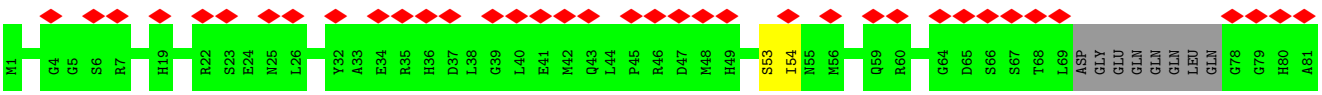
Chain Am:

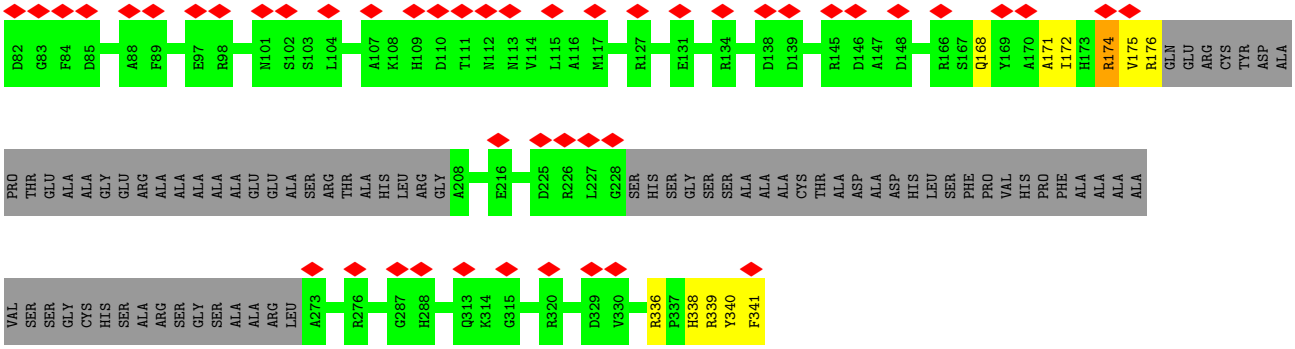




• Molecule 49: mL82

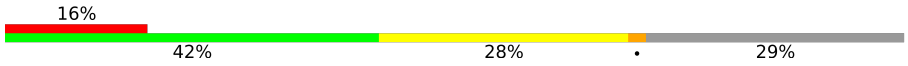
Chain Aq:

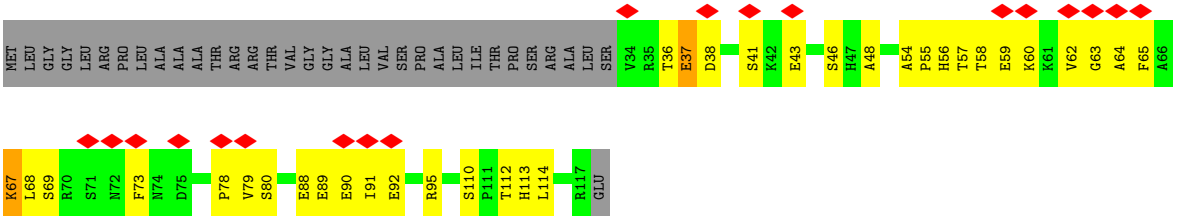




• Molecule 50: mL98

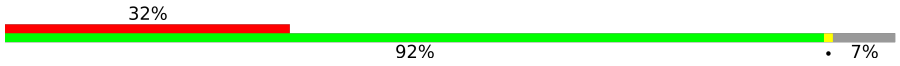
Chain BE:

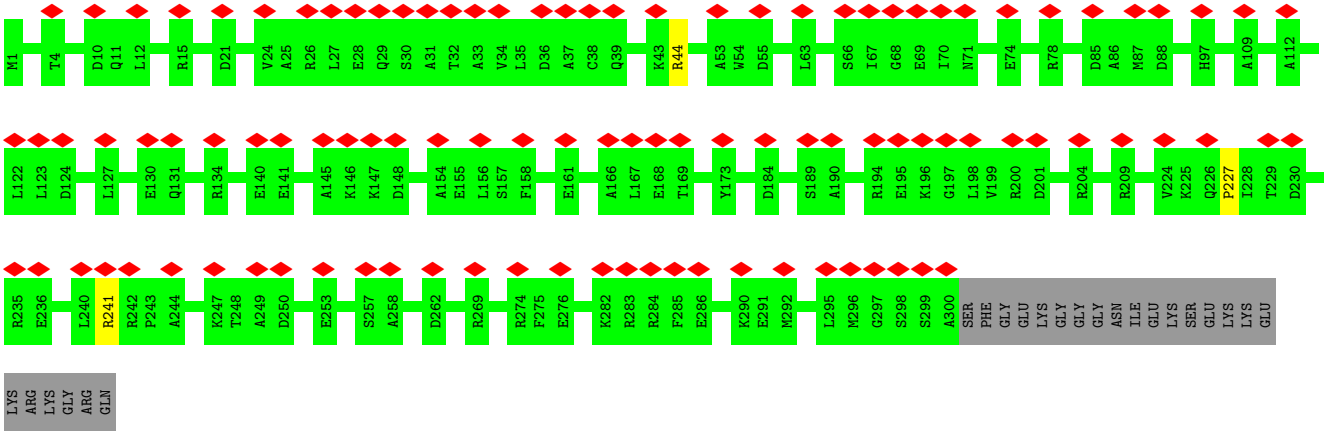




• Molecule 51: mL73

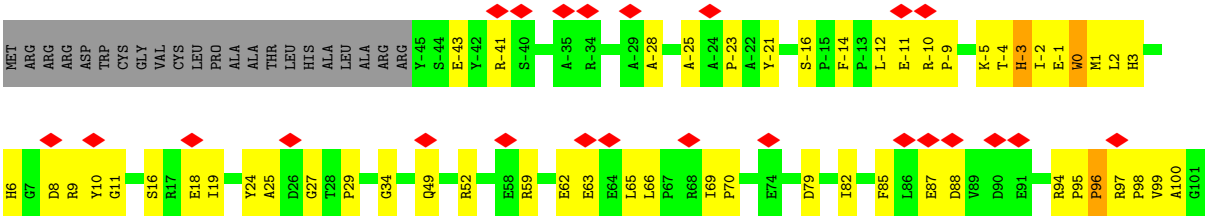
Chain Ak:

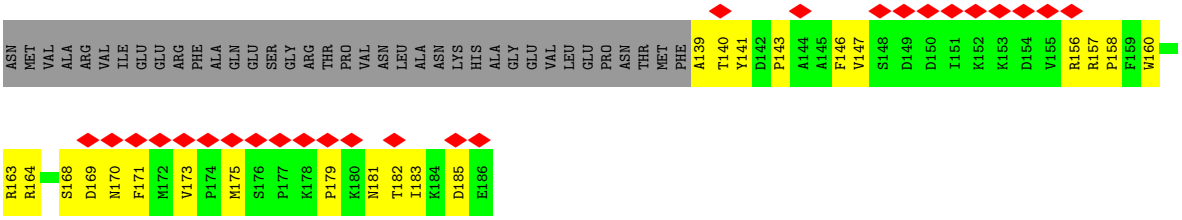




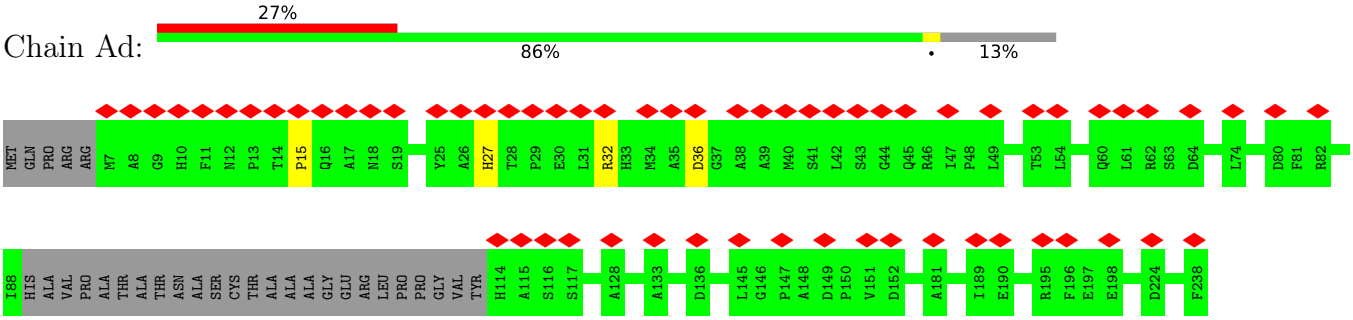
• Molecule 52: mL52,mL52

Chain BP:

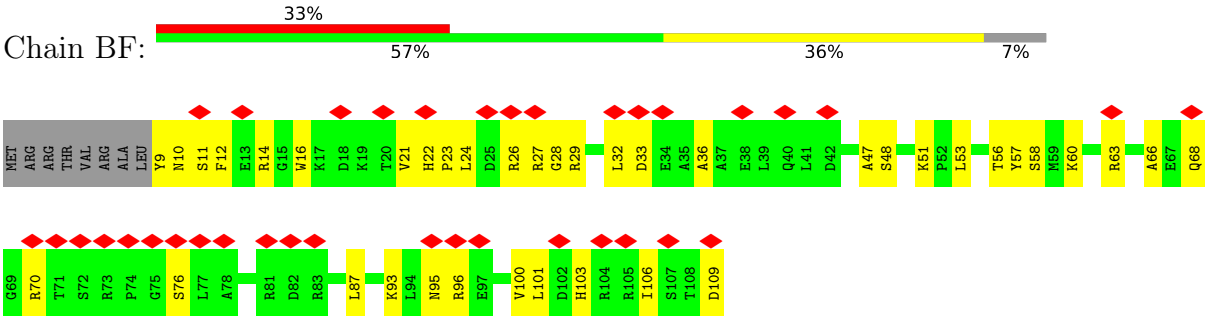




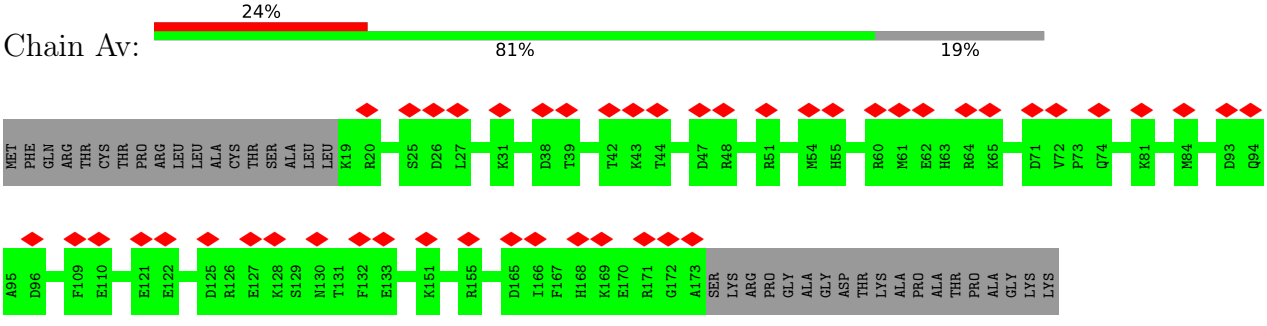
• Molecule 53: mL49



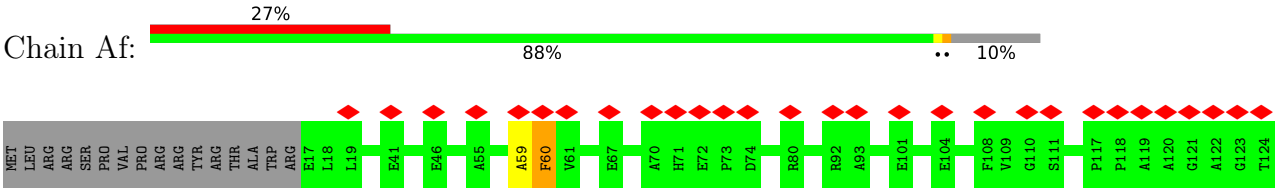
• Molecule 54: mL99

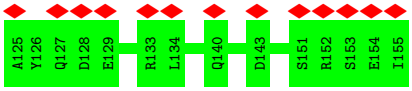


• Molecule 55: mL88



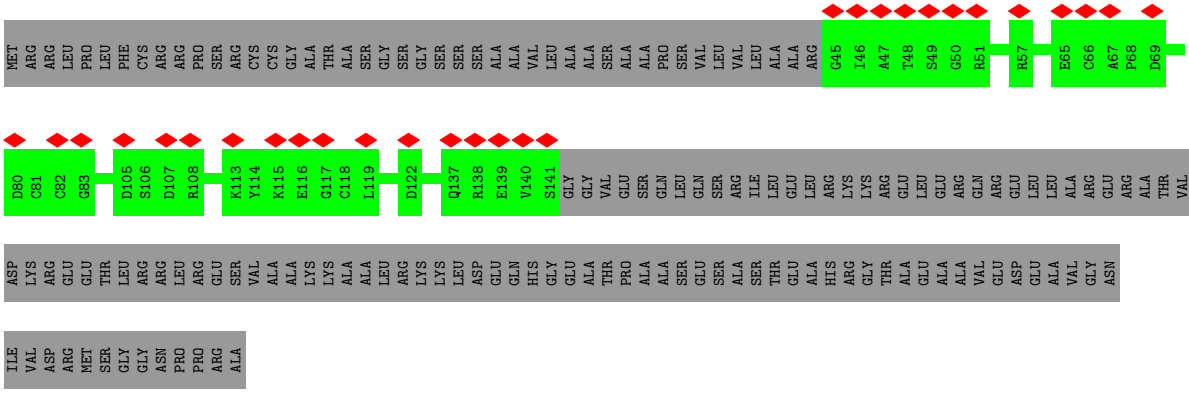
• Molecule 56: mL63





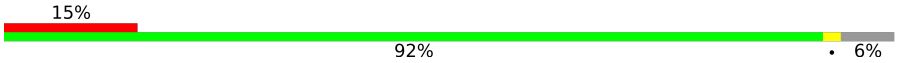
• Molecule 57: mL85

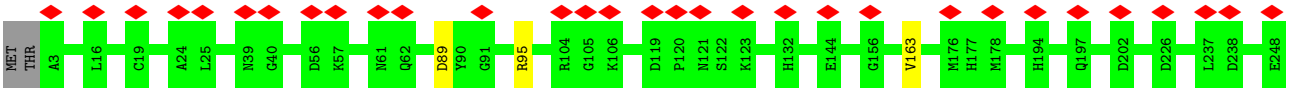
Chain As:

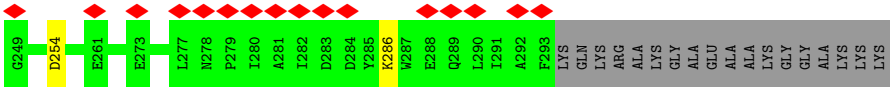


• Molecule 58: mL53

Chain Ae:

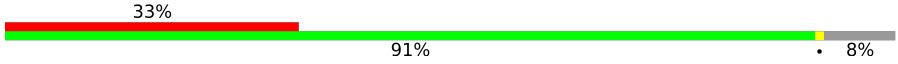


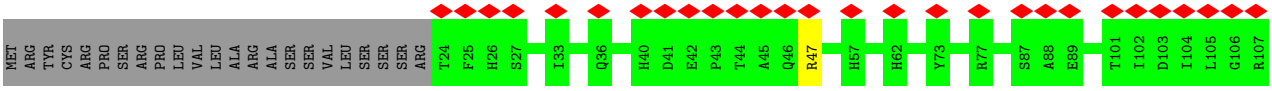


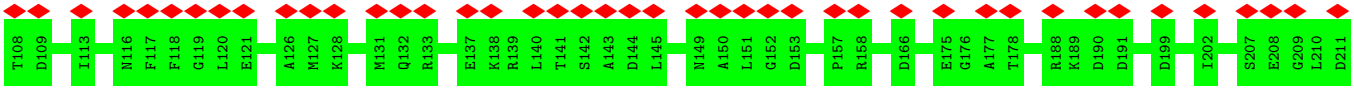


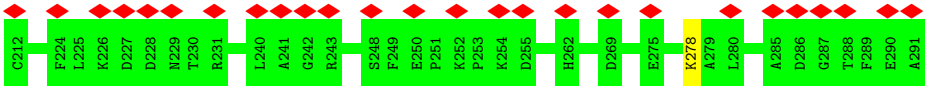
• Molecule 59: MRP-L46 domain-containing protein

Chain Ac:



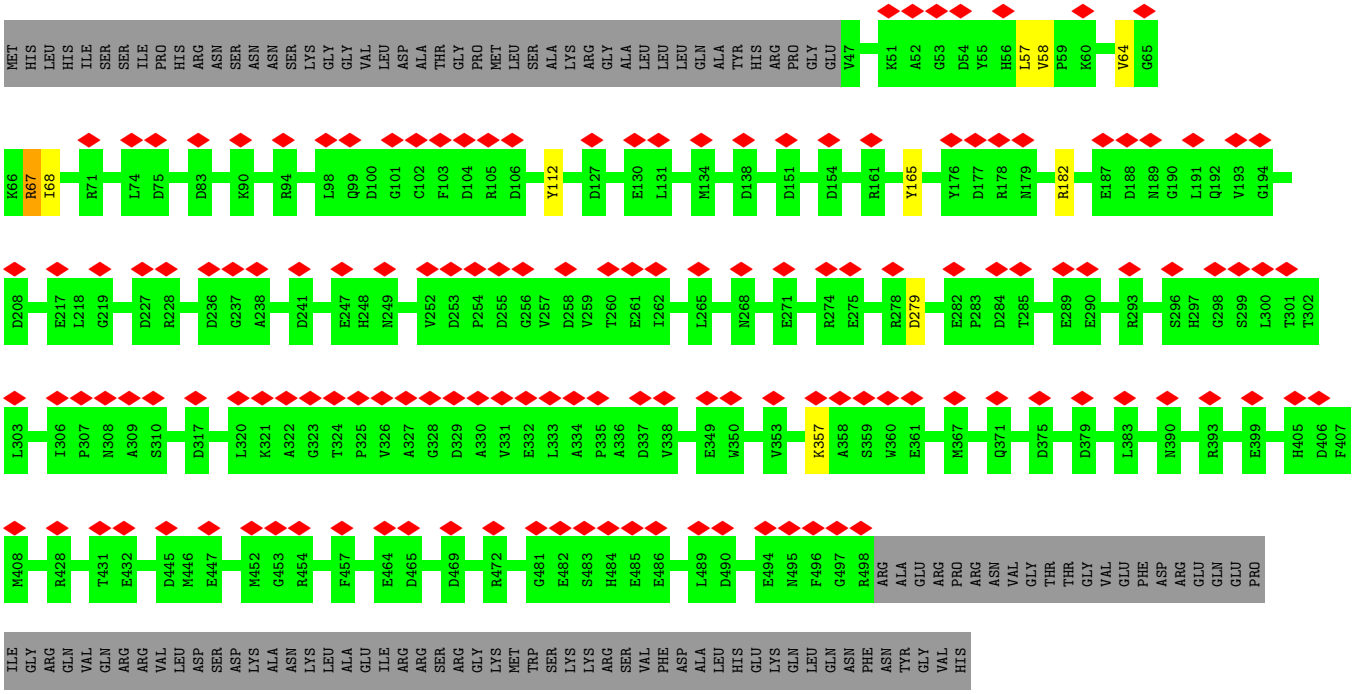






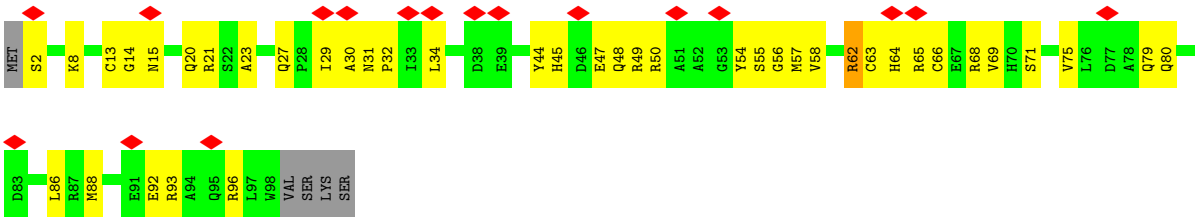
• Molecule 60: mL68

Chain Ah:



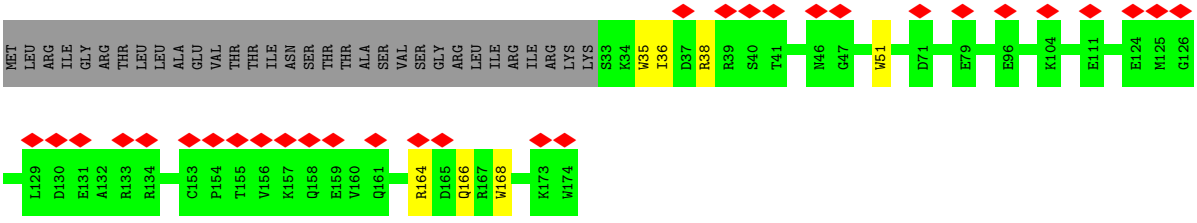
• Molecule 61: mL97

Chain BD:



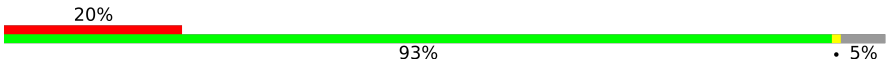
• Molecule 62: C2H2-type domain-containing protein

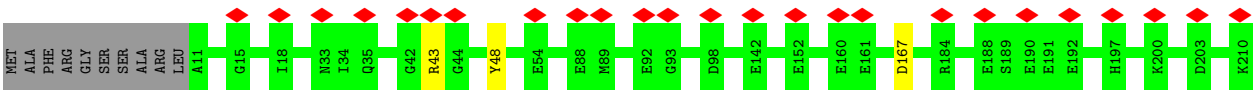
Chain Ay:

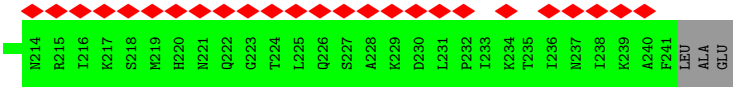


• Molecule 63: mL54/69

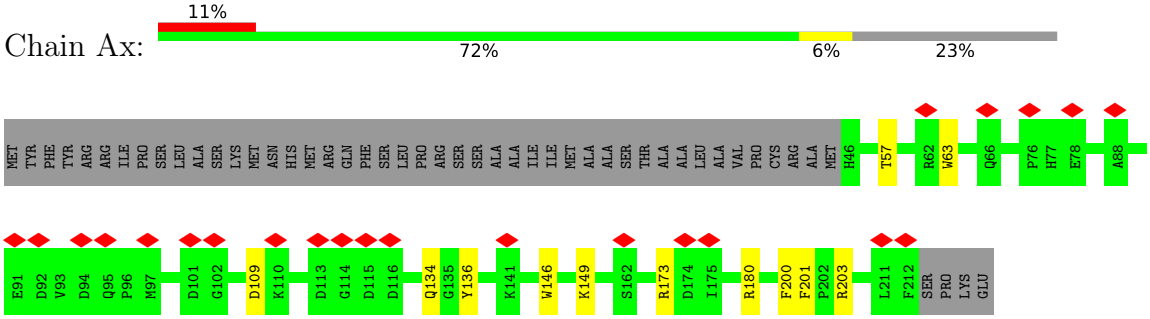
Chain Ag:



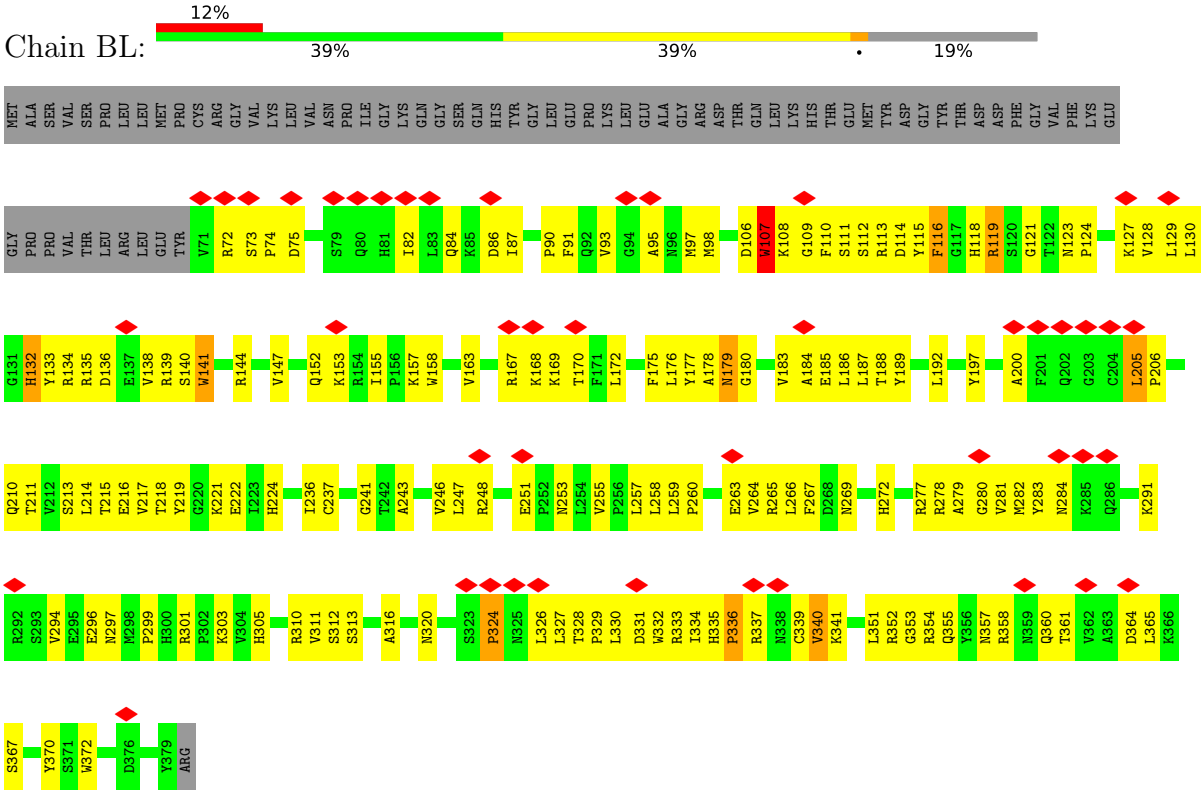




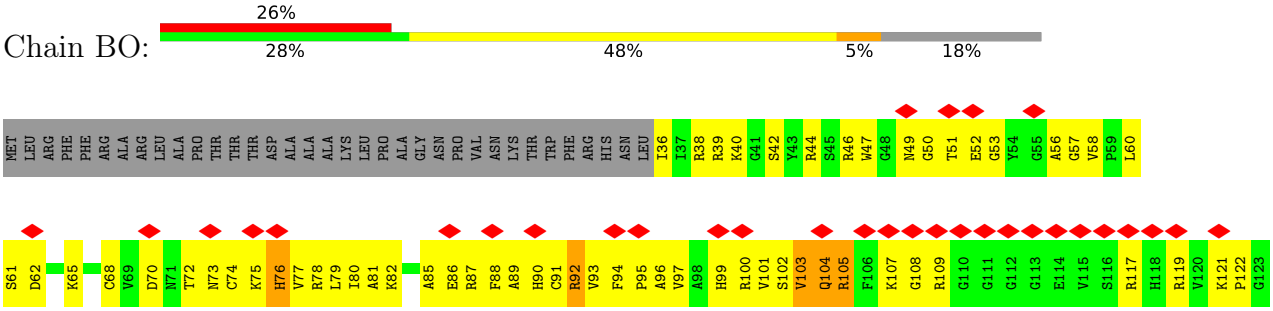
• Molecule 64: LIM zinc-binding domain-containing protein

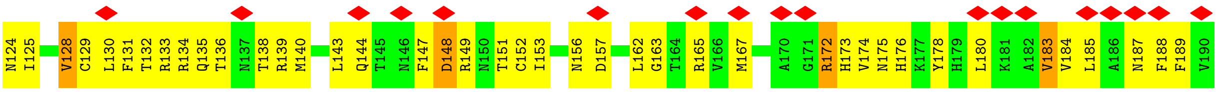


• Molecule 65: Putative ribosomal protein L2



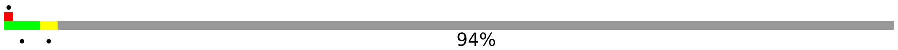
• Molecule 66: Putative ribosomal protein L14

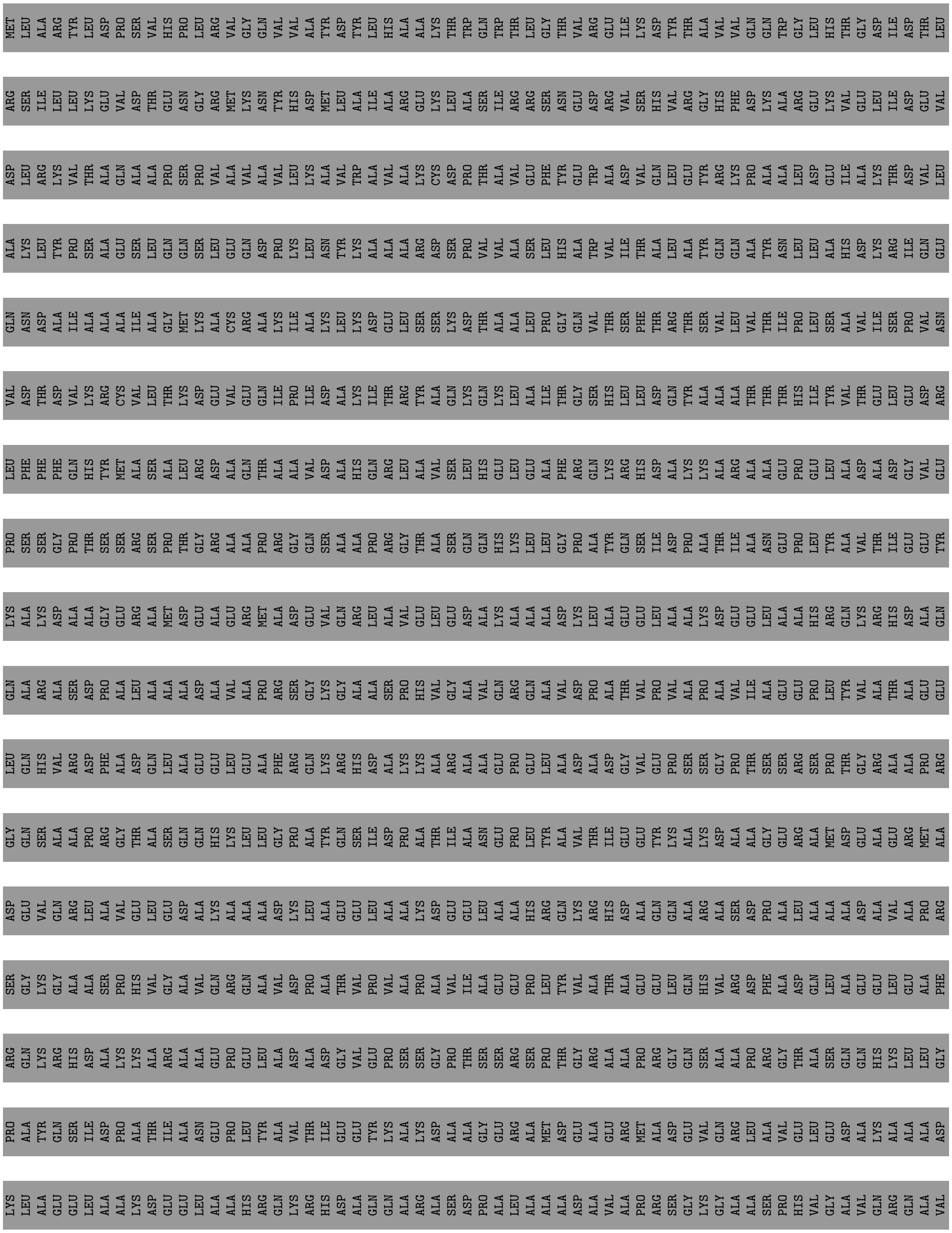


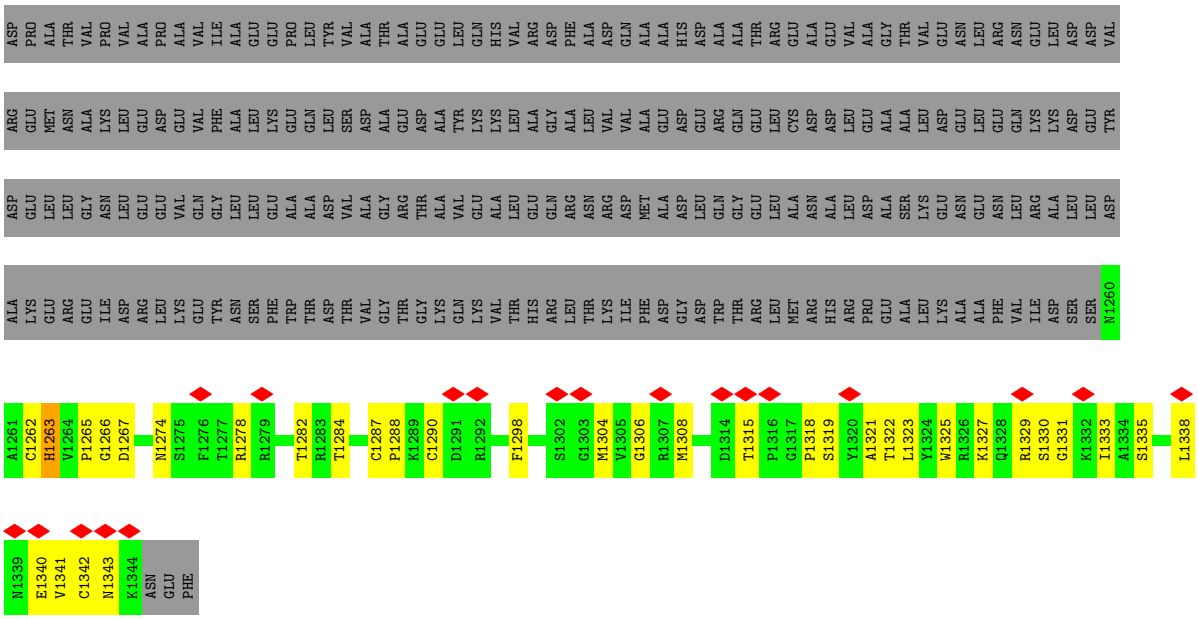


- Molecule 67: mL100

Chain BG:

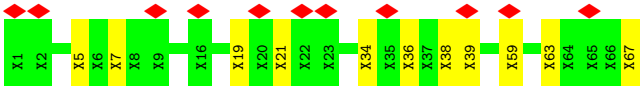






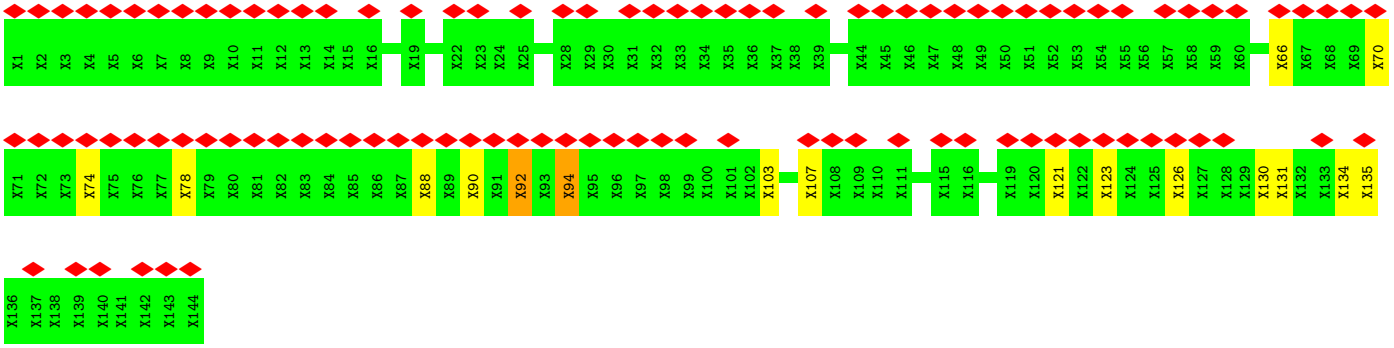
- Molecule 68: UB

Chain UB:



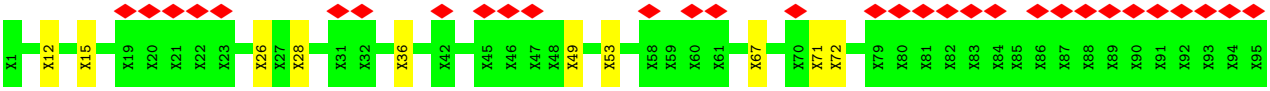
- Molecule 69: UC

Chain UC:



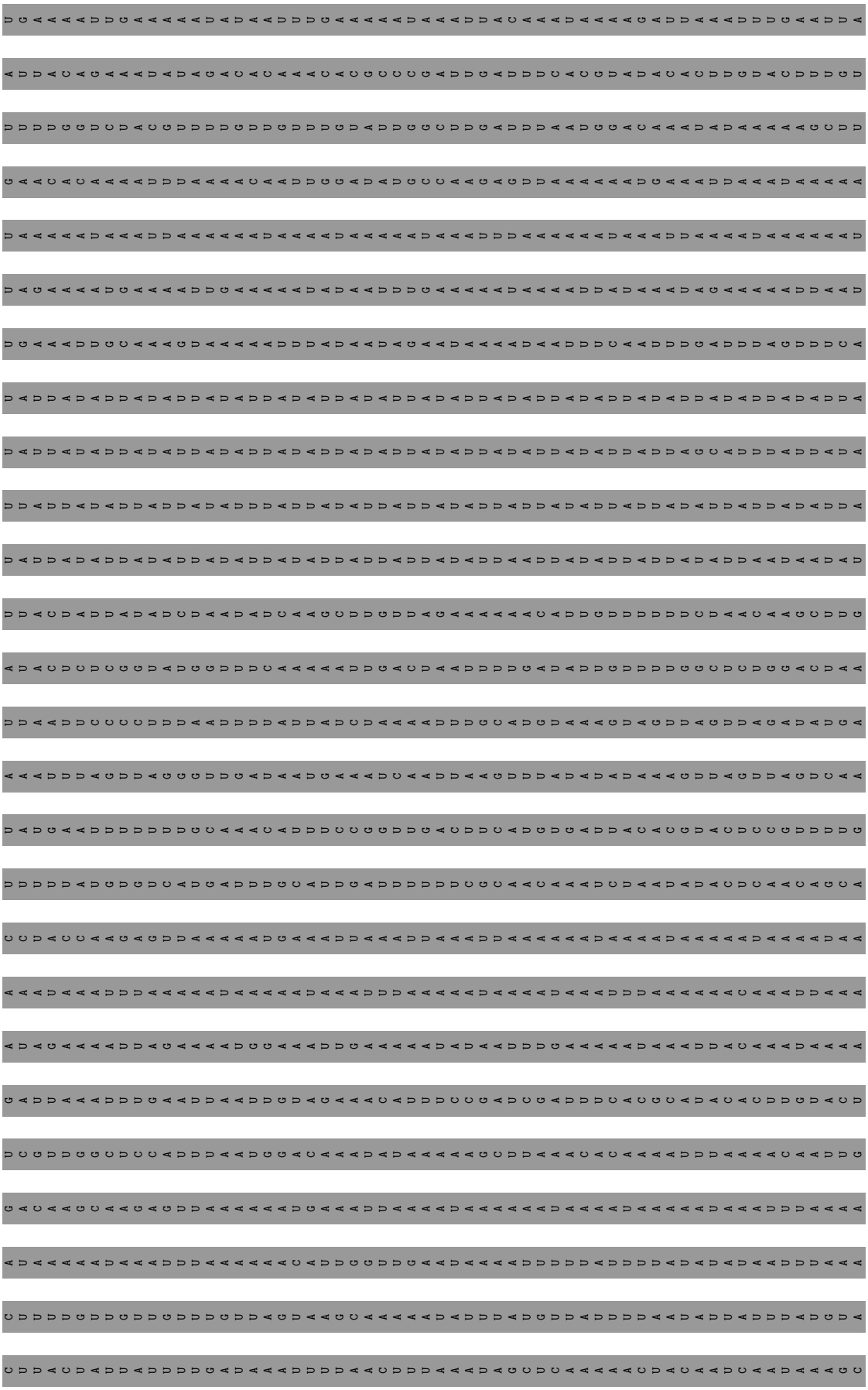
- Molecule 70: UD

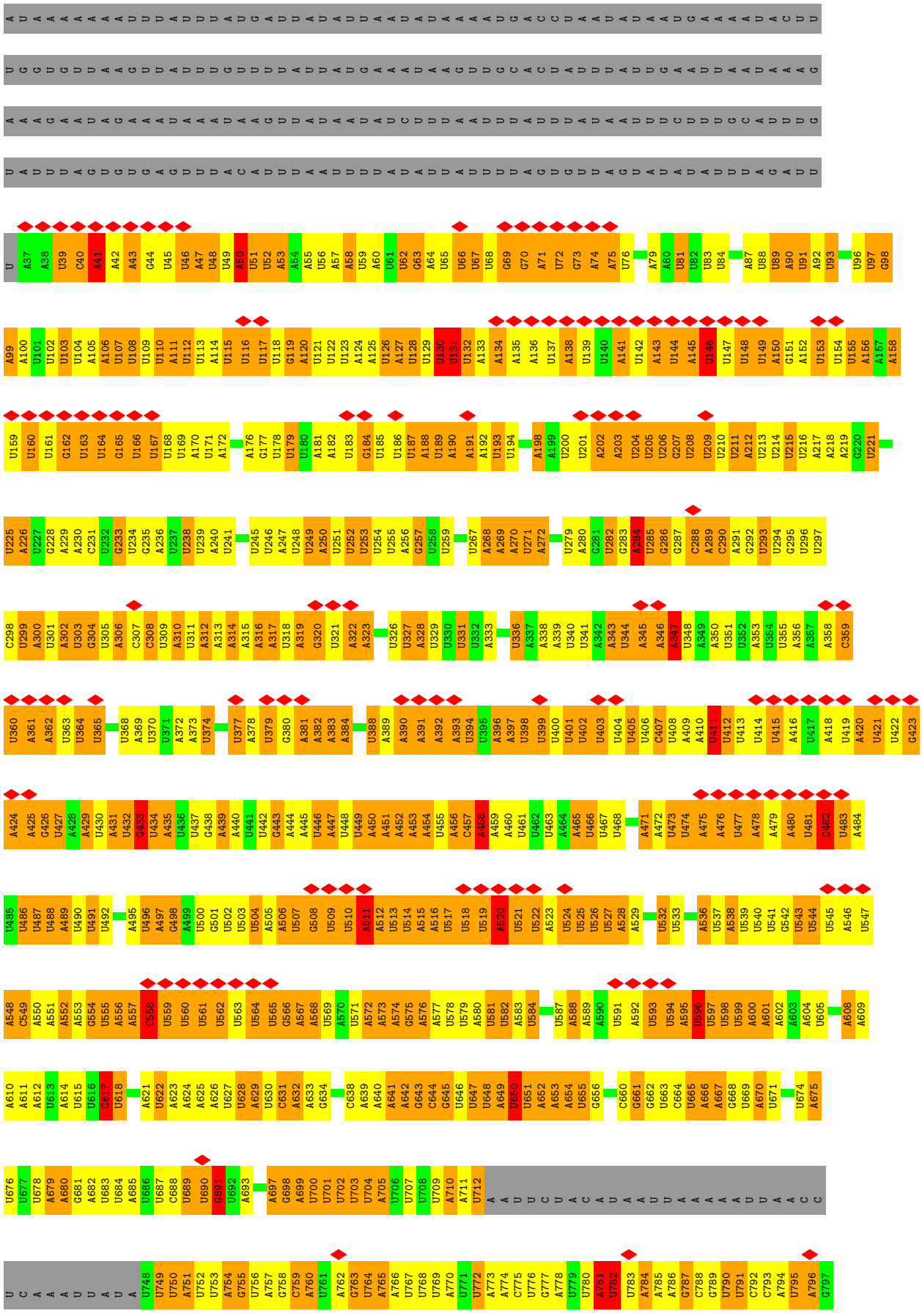
Chain UD:

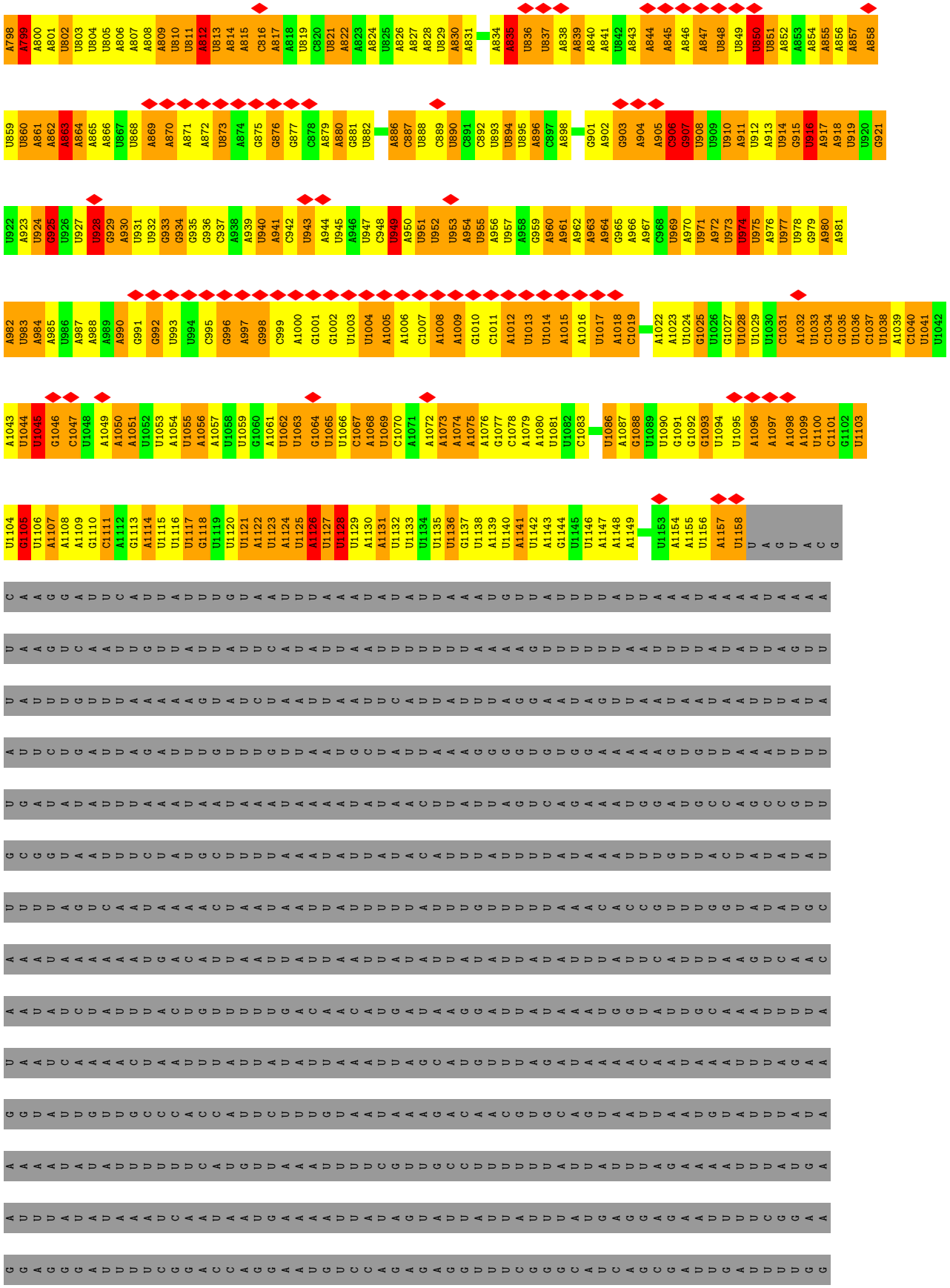


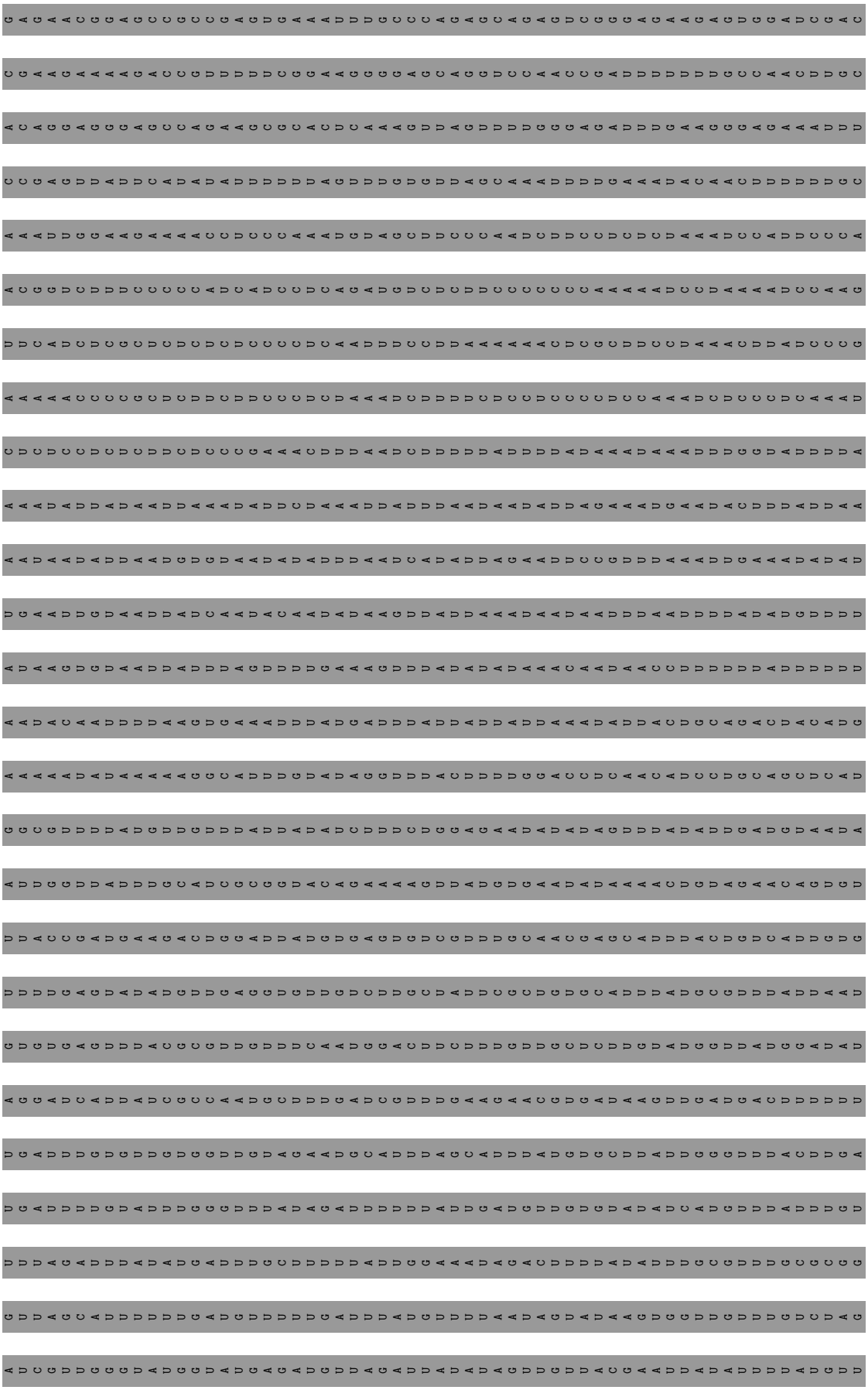
- Molecule 71: Ribosomal RNA

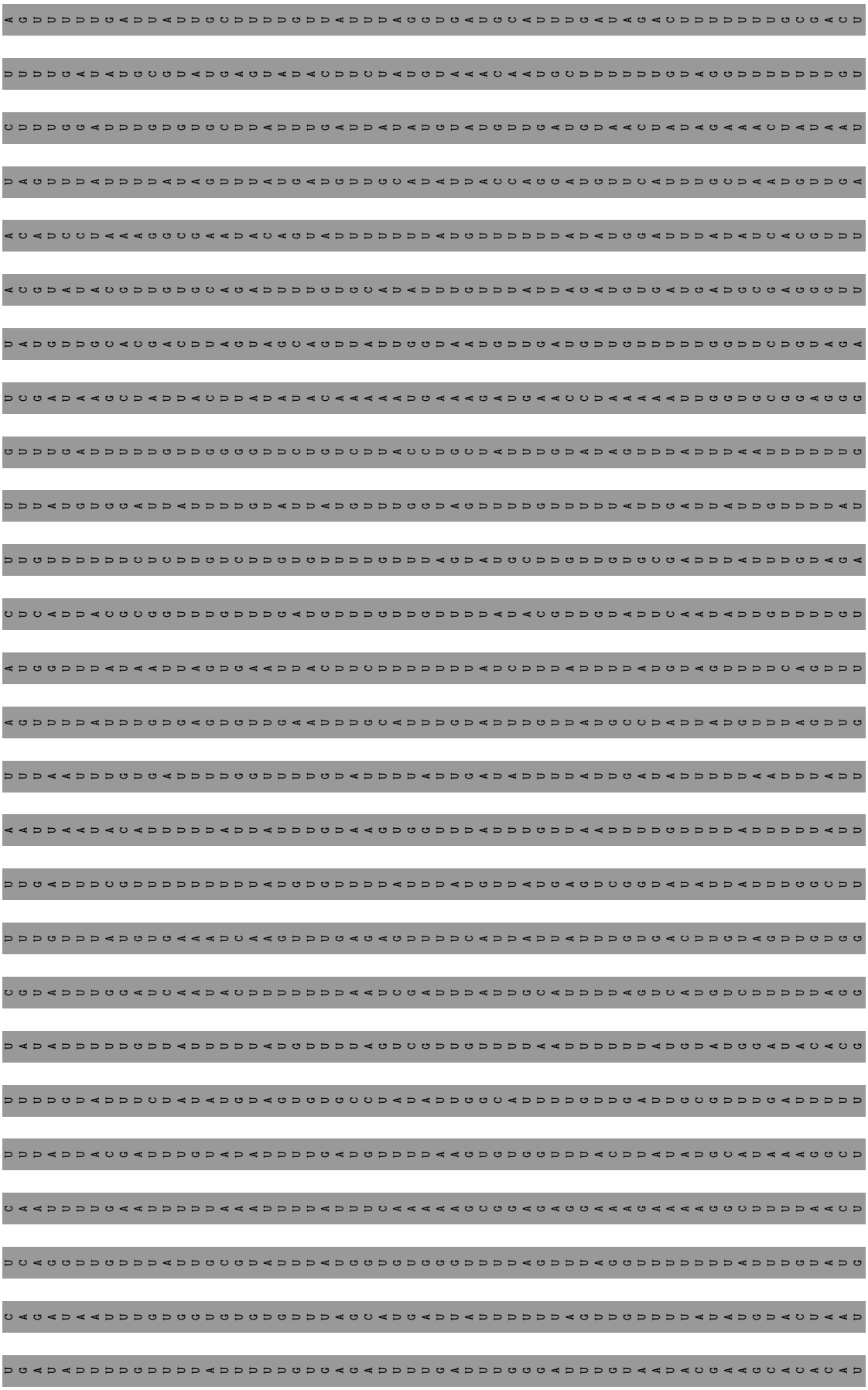
Chain 1:

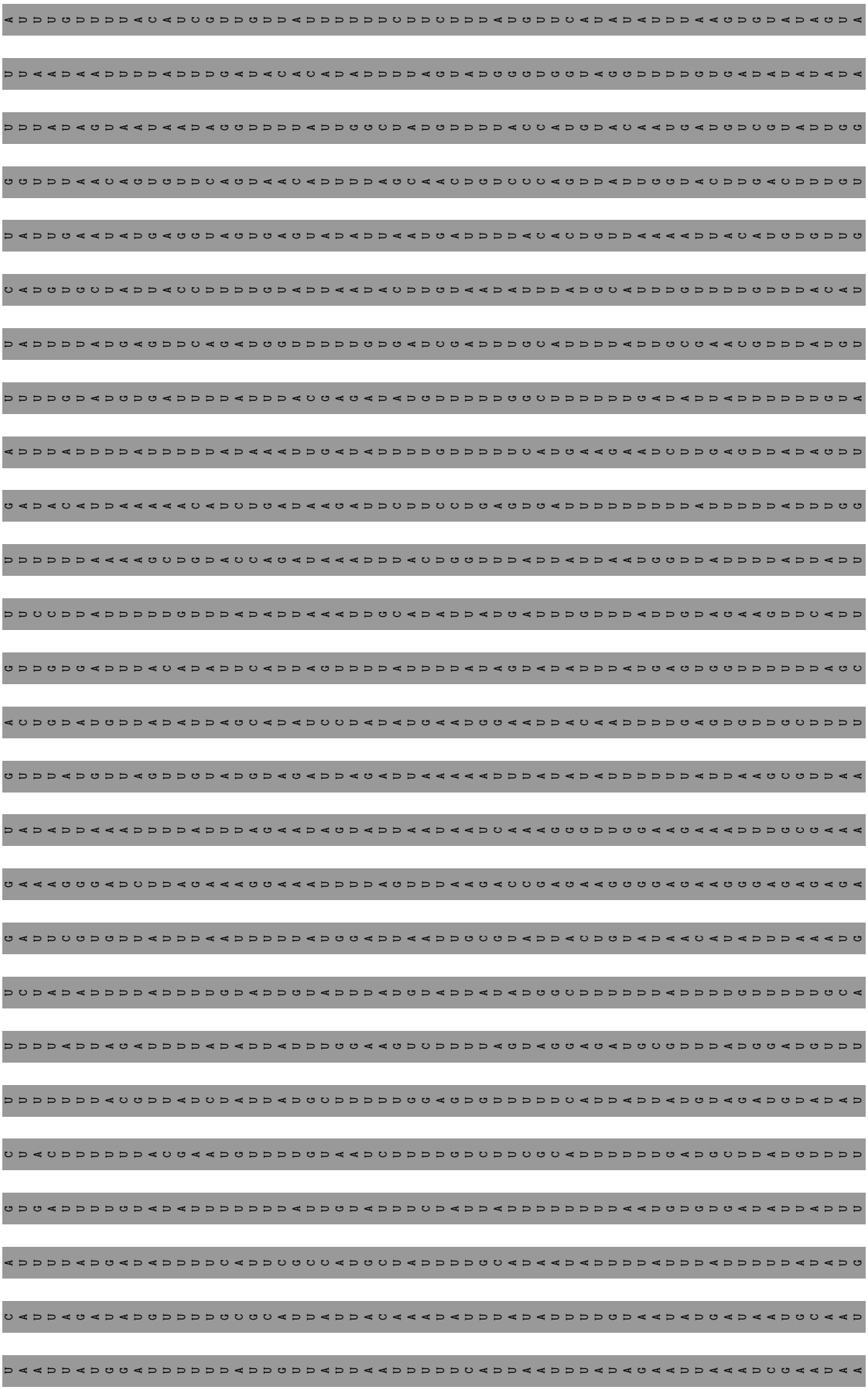


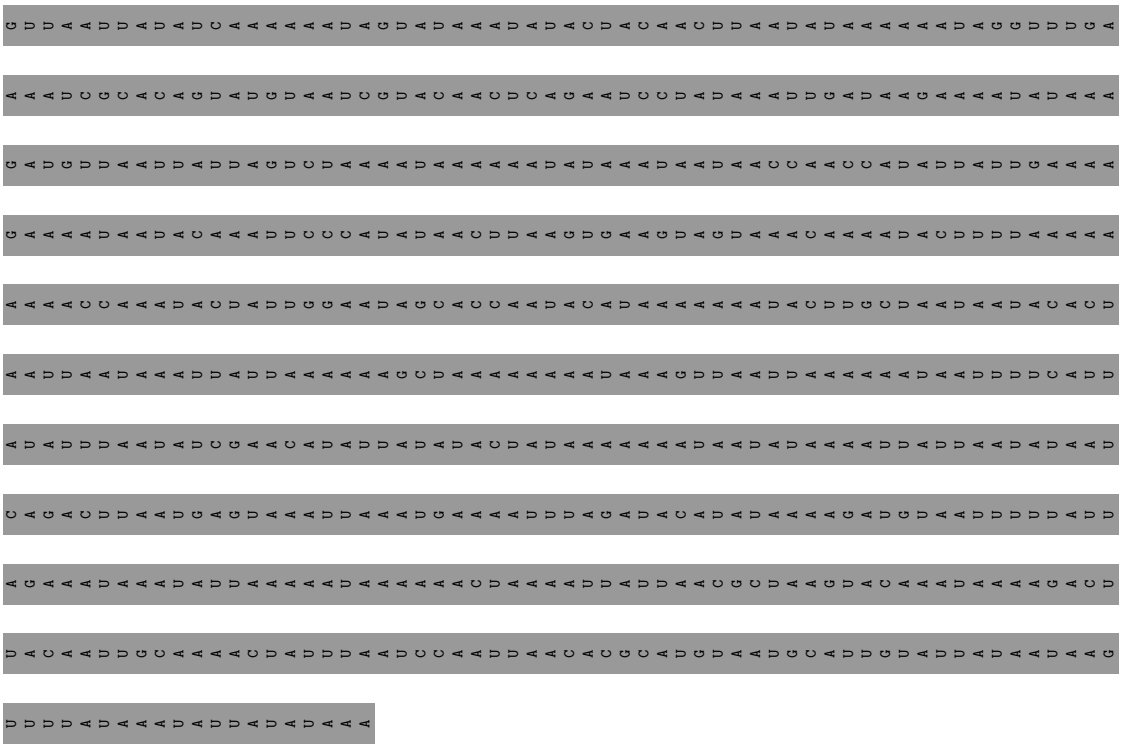












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.245	Depositor
Minimum map value	-0.135	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	476.00003, 476.00003, 476.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.58	0/3098	0.56	1/4217 (0.0%)
2	B	0.52	0/3623	0.54	1/4931 (0.0%)
3	C	0.52	0/1831	0.53	0/2498
4	D	0.45	0/1062	0.56	0/1438
5	E	0.46	0/2734	0.57	0/3687
6	F	0.53	0/1485	0.59	1/2019 (0.0%)
7	G	0.51	0/3110	0.61	2/4223 (0.0%)
8	H	0.46	0/1338	0.57	0/1808
9	I	0.50	0/2220	0.53	0/2998
10	J	0.48	0/1175	0.61	1/1582 (0.1%)
11	K	0.46	0/1499	0.50	0/2026
12	L	0.52	0/1452	0.55	0/1970
13	M	0.50	0/2168	0.60	2/2928 (0.1%)
14	N	0.55	0/1650	0.51	0/2242
15	O	0.42	0/2591	0.53	0/3507
16	P	0.51	0/1402	0.52	0/1892
17	Q	0.51	0/1827	0.54	0/2463
18	R	0.46	0/3852	0.54	1/5243 (0.0%)
19	S	0.48	0/1271	0.50	0/1712
20	T	0.51	0/501	0.49	0/665
21	U	0.49	0/756	0.74	1/1011 (0.1%)
22	V	0.53	0/1231	0.57	0/1645
23	W	0.51	0/483	0.69	0/657
24	X	0.49	0/3846	0.58	3/5250 (0.1%)
25	Y	0.41	0/2116	0.48	0/2866
26	Z	0.53	0/1268	0.69	0/1725
27	BA	0.42	0/1056	0.59	0/1435
29	BB	0.53	0/1061	0.62	0/1438
30	Aw	0.50	0/1552	0.52	0/2107
31	Bj	0.45	0/1389	0.50	0/1878
32	An	0.47	0/2677	0.65	0/3633
33	Al	0.49	0/2212	0.56	0/3013

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	BI	0.42	0/1440	0.53	0/1953
35	Az	0.61	0/1259	0.55	0/1700
36	At	0.45	0/1373	0.51	1/1848 (0.1%)
37	BC	0.38	0/1135	0.51	0/1532
38	Ab	0.48	0/2249	0.49	0/3044
39	Ai	0.48	0/3879	0.51	0/5258
40	Ap	0.40	0/1819	0.47	0/2458
41	Au	0.53	0/1542	0.65	0/2082
42	Aa	0.52	1/1454 (0.1%)	0.71	4/1968 (0.2%)
43	Ao	0.52	0/2351	0.56	0/3196
44	BM	0.31	0/3136	0.53	1/4259 (0.0%)
45	Ar	0.55	0/1689	0.55	0/2280
46	Aj	0.47	0/2826	0.50	0/3807
47	BH	0.50	0/1700	0.53	0/2301
48	Am	0.48	0/2791	0.52	1/3775 (0.0%)
49	Aq	0.45	0/2128	0.61	1/2876 (0.0%)
50	BE	0.47	0/723	0.63	0/981
51	Ak	0.38	0/2403	0.50	0/3265
52	BP	0.48	0/1648	0.60	1/2238 (0.0%)
53	Ad	0.52	0/1682	0.60	0/2283
54	BF	0.47	0/871	0.52	0/1170
55	Av	0.40	0/1335	0.48	0/1797
56	Af	0.47	0/1165	0.71	3/1585 (0.2%)
57	As	0.42	0/804	0.53	0/1093
58	Ae	0.48	0/2441	0.51	0/3324
59	Ac	0.41	0/2236	0.49	0/3038
60	Ah	0.44	0/3780	0.54	0/5125
61	BD	0.50	0/826	0.48	0/1109
62	Ay	0.51	0/1269	0.58	0/1724
63	Ag	0.52	0/1968	0.52	0/2661
64	Ax	0.56	0/1439	0.82	3/1952 (0.2%)
65	BL	0.53	0/2572	0.67	3/3482 (0.1%)
66	BO	0.49	0/1266	0.68	0/1702
67	BG	0.46	0/657	0.70	0/888
71	1	0.91	9/25626 (0.0%)	1.08	102/39842 (0.3%)
All	All	0.58	10/147018 (0.0%)	0.70	133/204303 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
9	I	0	1
12	L	0	1
18	R	0	1
26	Z	0	1
27	BA	0	2
28	UA	0	2
29	BB	0	2
31	Bj	0	1
32	An	0	2
41	Au	0	3
43	Ao	0	1
48	Am	0	1
49	Aq	0	2
50	BE	0	3
51	Ak	0	1
53	Ad	0	1
56	Af	0	1
65	BL	0	3
66	BO	0	5
69	UC	0	2
70	UD	0	1
All	All	0	38

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	Aa	193	TYR	N-CA	10.00	1.66	1.46
71	1	654	A	N9-C4	-7.40	1.33	1.37
71	1	886	A	N9-C4	-6.49	1.33	1.37
71	1	799	A	N9-C4	-5.76	1.34	1.37
71	1	814	A	N9-C4	-5.70	1.34	1.37
71	1	898	A	N9-C4	-5.67	1.34	1.37
71	1	880	A	N9-C4	-5.39	1.34	1.37
71	1	861	A	N9-C4	-5.38	1.34	1.37
71	1	863	A	N9-C4	-5.26	1.34	1.37
71	1	482	C	C1'-N1	5.26	1.56	1.48

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
71	1	146	U	N1-C1'-C2'	-11.88	98.56	114.00
56	Af	60	PHE	N-CA-C	-10.81	81.82	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	BP	-3	HIS	CB-CA-C	10.28	130.95	110.40
71	1	359	C	C2-N1-C1'	9.27	129.00	118.80
56	Af	59	ALA	N-CA-C	-8.93	86.89	111.00
71	1	347	A	N1-C6-N6	8.81	123.89	118.60
56	Af	59	ALA	CB-CA-C	8.47	122.81	110.10
42	Aa	91	LEU	N-CA-C	-8.46	88.17	111.00
71	1	359	C	N1-C2-O2	8.38	123.93	118.90
7	G	214	PRO	N-CA-C	-7.99	91.32	112.10
71	1	411	U	C2-N1-C1'	7.86	127.13	117.70
64	Ax	200	PHE	CB-CA-C	7.66	125.72	110.40
42	Aa	91	LEU	N-CA-CB	7.54	125.48	110.40
71	1	286	G	N3-C4-C5	7.37	132.29	128.60
71	1	1105	G	C6-C5-N7	-7.30	126.02	130.40
13	M	14	PRO	N-CA-CB	-7.26	94.59	103.30
71	1	347	A	C6-C5-N7	-7.21	127.26	132.30
71	1	359	C	C6-N1-C1'	-7.10	112.28	120.80
71	1	282	U	C4'-C3'-O3'	-7.09	94.52	109.40
71	1	112	U	C2-N1-C1'	7.04	126.15	117.70
71	1	286	G	N3-C4-N9	-7.03	121.78	126.00
6	F	158	PRO	N-CA-C	-7.02	93.84	112.10
24	X	353	PRO	CA-N-CD	-6.97	101.74	111.50
71	1	921	G	N3-C4-N9	-6.95	121.83	126.00
71	1	1045	U	N3-C2-O2	-6.89	117.38	122.20
71	1	41	A	N9-C1'-C2'	-6.83	104.49	112.00
1	A	290	MET	CB-CA-C	6.78	123.96	110.40
71	1	974	U	C2-N1-C1'	6.66	125.69	117.70
71	1	286	G	C2-N3-C4	-6.63	108.58	111.90
24	X	353	PRO	N-CA-CB	-6.60	95.34	102.60
7	G	149	PRO	N-CA-CB	-6.56	95.39	102.60
48	Am	324	ILE	C-N-CA	6.53	138.01	121.70
71	1	782	U	N1-C2-O2	6.51	127.36	122.80
71	1	359	C	C5-C6-N1	6.48	124.24	121.00
10	J	66	PRO	N-CA-CB	-6.43	95.52	102.60
71	1	347	A	O4'-C1'-N9	-6.39	103.09	108.20
71	1	347	A	C4-C5-N7	6.34	113.87	110.70
42	Aa	192	LEU	C-N-CA	6.29	137.43	121.70
71	1	925	G	N7-C8-N9	6.27	116.24	113.10
71	1	554	G	O4'-C1'-N9	6.26	113.21	108.20
71	1	411	U	N1-C2-O2	6.25	127.17	122.80
71	1	861	A	C2-N3-C4	-6.24	107.48	110.60
71	1	1045	U	N1-C2-O2	6.22	127.15	122.80
71	1	816	C	N1-C2-O2	6.22	122.63	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
71	1	1105	G	N1-C2-N2	-6.19	110.63	116.20
65	BL	107	TRP	CB-CA-C	6.16	122.72	110.40
71	1	1045	U	C2-N1-C1'	6.13	125.05	117.70
71	1	974	U	N3-C2-O2	-6.12	117.92	122.20
64	Ax	201	PHE	CB-CA-C	-6.11	98.18	110.40
71	1	782	U	C2-N1-C1'	6.04	124.95	117.70
71	1	284	A	OP1-P-O3'	6.00	118.40	105.20
71	1	1105	G	C2-N3-C4	-5.92	108.94	111.90
71	1	1105	G	C4-N9-C1'	5.92	134.19	126.50
71	1	179	U	N1-C2-O2	5.91	126.94	122.80
71	1	654	A	C2-N3-C4	-5.87	107.67	110.60
71	1	411	U	N3-C2-O2	-5.85	118.10	122.20
71	1	179	U	C2-N1-C1'	5.83	124.70	117.70
71	1	50	A	P-O3'-C3'	5.82	126.69	119.70
71	1	433	G	N9-C4-C5	-5.82	103.07	105.40
71	1	974	U	N1-C2-O2	5.82	126.87	122.80
71	1	921	G	N3-C4-C5	5.81	131.50	128.60
71	1	433	G	C4-C5-N7	5.81	113.12	110.80
71	1	458	A	N7-C8-N9	5.80	116.70	113.80
71	1	1105	G	N7-C8-N9	5.79	116.00	113.10
71	1	347	A	C5-C6-N6	-5.79	119.07	123.70
71	1	1105	G	N1-C2-N3	5.77	127.36	123.90
71	1	415	U	P-O3'-C3'	5.76	126.62	119.70
71	1	928	U	P-O3'-C3'	5.76	126.61	119.70
71	1	347	A	N9-C4-C5	-5.75	103.50	105.80
71	1	855	A	N1-C2-N3	5.70	132.15	129.30
71	1	816	C	N3-C2-O2	-5.68	117.92	121.90
71	1	835	A	P-O3'-C3'	5.68	126.51	119.70
71	1	558	C	C2-N1-C1'	5.67	125.04	118.80
71	1	782	U	N3-C2-O2	-5.66	118.24	122.20
71	1	906	C	C4'-C3'-O3'	-5.66	97.52	109.40
71	1	781	A	P-O3'-C3'	5.65	126.48	119.70
71	1	814	A	C2-N3-C4	-5.65	107.78	110.60
71	1	650	U	C2-N1-C1'	5.63	124.46	117.70
21	U	37	ASN	CB-CA-C	5.59	121.59	110.40
71	1	1126	A	P-O3'-C3'	5.59	126.41	119.70
71	1	130	U	N1-C2-O2	5.55	126.68	122.80
49	Aq	340	TYR	CB-CA-C	5.54	121.47	110.40
71	1	347	A	C5-N7-C8	-5.53	101.13	103.90
71	1	916	U	OP1-P-O3'	5.52	117.35	105.20
71	1	916	U	P-O3'-C3'	5.52	126.32	119.70
71	1	1128	U	P-O3'-C3'	5.51	126.31	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	ASP	CB-CG-OD1	5.47	123.23	118.30
71	1	50	A	OP1-P-O3'	5.45	117.19	105.20
71	1	1128	U	OP2-P-O3'	5.42	117.12	105.20
71	1	112	U	N1-C2-O2	5.42	126.59	122.80
18	R	395	LYS	CB-CA-C	-5.41	99.58	110.40
24	X	353	PRO	CB-CA-C	5.40	125.50	112.00
71	1	554	G	C6-C5-N7	-5.38	127.17	130.40
71	1	554	G	C4-N9-C1'	5.38	133.49	126.50
71	1	130	U	N3-C2-O2	-5.37	118.44	122.20
13	M	56	SER	CB-CA-C	-5.36	99.92	110.10
71	1	925	G	C8-N9-C4	-5.31	104.27	106.40
71	1	115	U	N1-C2-O2	5.31	126.52	122.80
44	BM	271	ARG	CB-CA-C	5.30	121.01	110.40
71	1	131	U	P-O3'-C3'	5.30	126.06	119.70
71	1	1114	A	N1-C2-N3	5.30	131.95	129.30
71	1	943	U	C2-N1-C1'	5.29	124.05	117.70
71	1	1044	U	N3-C2-O2	-5.29	118.50	122.20
71	1	949	U	N3-C2-O2	-5.28	118.50	122.20
71	1	691	G	N3-C4-C5	5.28	131.24	128.60
36	At	165	GLU	C-N-CA	5.28	134.89	121.70
71	1	855	A	C2-N3-C4	-5.25	107.98	110.60
71	1	433	G	O4'-C1'-N9	5.23	112.39	108.20
71	1	284	A	P-O3'-C3'	5.23	125.98	119.70
71	1	812	A	OP2-P-O3'	5.22	116.70	105.20
71	1	850	U	O4'-C1'-N1	5.21	112.37	108.20
71	1	861	A	N1-C2-N3	5.21	131.91	129.30
71	1	596	U	P-O3'-C3'	5.20	125.94	119.70
71	1	520	A	O5'-P-OP1	-5.19	101.03	105.70
71	1	1131	A	C2-N3-C4	-5.18	108.01	110.60
71	1	112	U	N3-C2-O2	-5.18	118.58	122.20
71	1	286	G	N3-C2-N2	-5.17	116.28	119.90
71	1	654	A	N3-C4-C5	5.17	130.42	126.80
71	1	907	G	C4-C5-N7	5.16	112.86	110.80
71	1	390	A	N1-C2-N3	5.13	131.86	129.30
71	1	596	U	OP1-P-O3'	5.12	116.46	105.20
71	1	411	U	C6-N1-C1'	-5.11	114.04	121.20
71	1	617	G	N3-C4-C5	-5.11	126.04	128.60
71	1	759	C	P-O3'-C3'	5.11	125.83	119.70
71	1	359	C	N3-C2-O2	-5.09	118.33	121.90
71	1	816	C	C2-N1-C1'	5.09	124.40	118.80
64	Ax	149	LYS	CB-CA-C	5.09	120.58	110.40
71	1	1088	G	N3-C4-C5	5.08	131.14	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
71	1	1114	A	C2-N3-C4	-5.04	108.08	110.60
71	1	511	A	C4'-C3'-O3'	-5.03	98.83	109.40
65	BL	205	LEU	CA-CB-CG	5.02	126.85	115.30
65	BL	108	LYS	N-CA-C	-5.01	97.47	111.00
42	Aa	192	LEU	N-CA-CB	-5.01	100.38	110.40

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	Ad	36	ASP	Peptide
56	Af	60	PHE	Peptide
51	Ak	227	PRO	Peptide
48	Am	329	PRO	Peptide
32	An	49	SER	Peptide
32	An	50	HIS	Peptide
43	Ao	19	ARG	Peptide
49	Aq	171	ALA	Peptide
49	Aq	174	ARG	Peptide
41	Au	26	TYR	Peptide
41	Au	55	SER	Peptide
41	Au	61	PHE	Peptide
27	BA	139	THR	Peptide
27	BA	141	VAL	Peptide
29	BB	129	THR	Peptide
29	BB	55	GLN	Peptide
50	BE	69	SER	Peptide
50	BE	78	PRO	Peptide
50	BE	79	VAL	Peptide
65	BL	178	ALA	Peptide
65	BL	179	ASN	Peptide
65	BL	336	PRO	Peptide
66	BO	103	VAL	Peptide
66	BO	104	GLN	Peptide
66	BO	183	VAL	Peptide
66	BO	75	LYS	Peptide
66	BO	76	HIS	Peptide
31	Bj	101	PRO	Peptide
3	C	142	ASN	Peptide
9	I	235	TRP	Peptide
12	L	71	ARG	Peptide
18	R	125	PRO	Peptide

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Mol	Chain	Res	Type	Group
28	UA	47	UNK	Peptide
28	UA	81	UNK	Peptide
69	UC	92	UNK	Peptide
69	UC	94	UNK	Peptide
70	UD	67	UNK	Peptide
26	Z	21	PHE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2996	0	2807	124	0
2	B	3513	0	3413	129	0
3	C	1772	0	1734	71	0
4	D	1036	0	1038	28	0
5	E	2668	0	2697	94	0
6	F	1435	0	1396	63	0
7	G	3012	0	2917	125	0
8	H	1305	0	1315	82	0
9	I	2153	0	2089	133	0
10	J	1146	0	1145	81	0
11	K	1467	0	1469	59	0
12	L	1419	0	1443	50	0
13	M	2116	0	2150	122	0
14	N	1599	0	1591	75	0
15	O	2537	0	2530	131	0
16	P	1367	0	1374	70	0
17	Q	1785	0	1784	79	0
18	R	3755	0	3722	152	0
19	S	1244	0	1272	40	0
20	T	487	0	496	26	0
21	U	744	0	798	71	0
22	V	1202	0	1224	78	0
23	W	465	0	446	13	0
24	X	3733	0	3604	142	0
25	Y	2067	0	1955	67	0
26	Z	1223	0	1192	73	0
27	BA	1038	0	1052	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	UA	1015	0	213	22	0
29	BB	1028	0	1003	66	0
30	Aw	1509	0	1470	0	0
31	Bj	1358	0	1422	0	0
32	An	2605	0	2536	0	0
33	Al	2152	0	2112	0	0
34	BI	1409	0	1400	46	0
35	Az	1215	0	1144	0	0
36	At	1346	0	1299	0	0
37	BC	1114	0	1096	43	0
38	Ab	2185	0	2095	0	0
39	Ai	3789	0	3752	0	0
40	Ap	1775	0	1699	0	0
41	Au	1490	0	1450	0	0
42	Aa	1417	0	1377	0	0
43	Ao	2276	0	2176	0	0
44	BM	3069	0	3105	196	0
45	Ar	1644	0	1608	0	0
46	Aj	2766	0	2765	0	0
47	BH	1659	0	1607	64	0
48	Am	2708	0	2634	0	0
49	Aq	2074	0	2050	0	0
50	BE	700	0	665	35	0
51	Ak	2352	0	2369	0	0
52	BP	1593	0	1529	80	0
53	Ad	1632	0	1607	0	0
54	BF	851	0	831	41	0
55	Av	1300	0	1284	0	0
56	Af	1132	0	1108	0	0
57	As	787	0	777	0	0
58	Ae	2359	0	2328	0	0
59	Ac	2174	0	2096	0	0
60	Ah	3686	0	3572	0	0
61	BD	807	0	772	32	0
62	Ay	1226	0	1157	0	0
63	Ag	1916	0	1888	0	0
64	Ax	1388	0	1308	0	0
65	BL	2497	0	2489	163	0
66	BO	1239	0	1246	148	0
67	BG	643	0	617	24	0
68	UB	335	0	73	8	0
69	UC	720	0	151	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	UD	475	0	105	8	0
71	1	22918	0	11465	1051	0
72	Ax	2	0	0	0	0
72	BD	1	0	0	0	0
72	BG	1	0	0	2	0
72	T	1	0	0	2	0
72	W	1	0	0	0	0
73	Ag	44	0	26	0	0
All	All	143667	0	128129	3654	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (3654) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:25:PHE:HD1	71:1:933:G:N2	1.46	1.10
21:U:25:PHE:HB3	71:1:972:A:H61	1.09	1.09
21:U:39:VAL:HG21	21:U:85:GLU:HB2	1.36	1.03
10:J:67:ARG:HG2	10:J:68:PRO:HD2	1.38	1.02
10:J:67:ARG:CG	10:J:68:PRO:HD2	1.90	1.01
2:B:124:ASN:HB2	2:B:199:SER:HB3	1.38	1.00
21:U:25:PHE:CD1	71:1:933:G:N2	2.26	0.99
24:X:498:ARG:HG2	24:X:498:ARG:HH11	1.30	0.96
21:U:31:PRO:HB3	21:U:60:ARG:NH1	1.80	0.96
2:B:194:LYS:C	2:B:194:LYS:HE2	1.86	0.96
20:T:73:CYS:HG	72:T:101:ZN:ZN	0.73	0.95
71:1:924:U:HO2'	71:1:925:G:H8	0.96	0.95
24:X:320:VAL:HG13	24:X:393:CYS:HB3	1.49	0.94
9:I:175:LYS:H	9:I:201:ARG:HH12	1.14	0.94
10:J:67:ARG:CG	10:J:68:PRO:CD	2.46	0.94
21:U:25:PHE:CB	71:1:972:A:H61	1.81	0.93
71:1:863:A:N1	71:1:1105:G:N2	2.17	0.92
29:BB:111:PHE:CE1	29:BB:112:LEU:O	2.23	0.92
10:J:67:ARG:HG3	10:J:68:PRO:CD	1.99	0.92
6:F:161:GLN:HA	6:F:161:GLN:HE21	1.35	0.91
24:X:352:LYS:HB3	24:X:353:PRO:HD2	1.50	0.91
52:BP:97:ARG:N	52:BP:98:PRO:HD2	1.83	0.91
66:BO:172:ARG:HH21	66:BO:172:ARG:HA	1.34	0.91
24:X:499:ARG:HD2	47:BH:202:GLU:HG3	1.50	0.91
25:Y:247:TYR:HH	25:Y:258:TRP:HE1	1.03	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BM:31:ARG:HH22	44:BM:47:LYS:HG3	1.34	0.90
71:1:55:A:H61	71:1:122:U:H3	1.17	0.90
54:BF:96:ARG:NH2	71:1:563:U:O2'	2.04	0.90
10:J:67:ARG:HB2	10:J:67:ARG:NH2	1.87	0.90
65:BL:114:ASP:HB3	65:BL:130:LEU:HD13	1.55	0.89
8:H:27:ARG:HH22	8:H:96:LYS:HG2	1.37	0.89
5:E:121:THR:N	71:1:433:G:OP1	2.07	0.88
14:N:50:ARG:HH11	22:V:27:LYS:HG2	1.37	0.87
21:U:17:ARG:HD3	21:U:17:ARG:N	1.88	0.87
10:J:67:ARG:HG3	10:J:68:PRO:HD3	1.55	0.86
6:F:40:PRO:HB3	11:K:69:ALA:HB2	1.55	0.86
15:O:23:GLN:NE2	15:O:23:GLN:HA	1.90	0.86
24:X:358:GLU:HG2	24:X:364:PRO:HG2	1.57	0.86
17:Q:108:ILE:HB	71:1:905:A:H62	1.39	0.86
17:Q:108:ILE:HG23	17:Q:108:ILE:O	1.76	0.85
71:1:925:G:H1	71:1:931:U:H3	1.24	0.85
7:G:163:ARG:NH2	71:1:193:U:OP2	2.10	0.85
71:1:53:A:H61	71:1:124:A:H62	1.23	0.85
11:K:59:ARG:NH2	71:1:410:A:OP2	2.09	0.85
71:1:508:G:N2	71:1:518:U:OP1	2.08	0.85
22:V:76:MET:O	22:V:81:ARG:NH2	2.10	0.85
21:U:25:PHE:HB3	71:1:972:A:N6	1.90	0.85
16:P:48:GLU:HA	16:P:78:THR:HG22	1.58	0.85
18:R:281:GLU:HA	18:R:284:LYS:HG2	1.58	0.84
71:1:923:A:O2'	71:1:980:A:OP2	1.95	0.84
65:BL:93:VAL:HG11	65:BL:163:VAL:HG22	1.58	0.84
65:BL:119:ARG:HH11	65:BL:132:HIS:C	1.81	0.84
71:1:887:C:N3	71:1:979:G:N2	2.26	0.84
11:K:23:MET:SD	71:1:146:U:C4	2.70	0.84
65:BL:310:ARG:HH11	71:1:297:U:H3	1.21	0.84
71:1:40:C:H1'	71:1:41:A:N7	1.93	0.84
7:G:209:ARG:NH1	71:1:190:A:N3	2.25	0.84
24:X:367:GLN:HG2	24:X:384:LYS:HG3	1.60	0.83
2:B:291:TYR:OH	71:1:111:A:N6	2.11	0.83
29:BB:105:GLU:CD	29:BB:106:PRO:HD2	1.98	0.83
44:BM:45:SER:HA	44:BM:118:ILE:HG21	1.60	0.83
3:C:55:MET:SD	3:C:63:ARG:NH1	2.52	0.83
13:M:74:LYS:NZ	71:1:50:A:OP1	2.12	0.83
18:R:30:PRO:HD3	18:R:83:ARG:HG2	1.59	0.82
3:C:142:ASN:ND2	71:1:904:A:OP1	2.13	0.82
3:C:205:TYR:O	3:C:208:ARG:NH1	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:955:U:H5	71:1:970:A:H61	1.26	0.82
71:1:975:U:O2	71:1:975:U:H2'	1.79	0.82
15:O:28:ALA:HB1	15:O:29:ARG:HE	1.44	0.82
71:1:221:U:O2'	71:1:882:U:O2'	1.97	0.82
24:X:302:THR:O	24:X:306:ALA:N	2.10	0.81
15:O:29:ARG:H	15:O:29:ARG:HD2	1.46	0.81
14:N:76:TYR:OH	71:1:316:A:OP2	1.98	0.81
44:BM:128:LEU:HD12	44:BM:278:LEU:HB3	1.63	0.81
66:BO:86:GLU:OE2	66:BO:99:HIS:NE2	2.12	0.81
66:BO:103:VAL:HG11	66:BO:122:PRO:HA	1.63	0.81
14:N:95:TYR:OH	71:1:556:A:OP1	1.99	0.81
2:B:365:GLU:HG2	2:B:372:PRO:HA	1.61	0.81
71:1:933:G:H2'	71:1:934:G:C8	2.16	0.80
2:B:201:ARG:NH2	71:1:186:U:O4	2.13	0.80
26:Z:76:ARG:NH1	71:1:70:G:O3'	2.12	0.80
67:BG:1319:SER:HB2	67:BG:1322:THR:HG22	1.64	0.80
7:G:10:ARG:NH1	71:1:486:U:OP1	2.15	0.80
12:L:29:ASN:ND2	52:BP:10:TYR:OH	2.09	0.80
17:Q:31:ILE:HD12	61:BD:32:PRO:HB3	1.63	0.80
44:BM:192:LEU:HD11	44:BM:252:VAL:HG22	1.63	0.80
52:BP:-3:HIS:O	52:BP:1:MET:HG3	1.82	0.80
21:U:39:VAL:CG2	21:U:85:GLU:HB2	2.11	0.80
44:BM:377:GLU:HG2	44:BM:381:ASN:HD21	1.47	0.80
21:U:25:PHE:CB	71:1:933:G:H21	1.95	0.80
19:S:343:ARG:NH2	71:1:368:U:OP2	2.15	0.80
2:B:148:ARG:O	14:N:85:ARG:NH1	2.15	0.80
27:BA:69:ILE:HG22	27:BA:88:VAL:HB	1.64	0.80
18:R:167:HIS:HD2	18:R:169:GLY:H	1.30	0.79
29:BB:111:PHE:CD1	29:BB:111:PHE:C	2.55	0.79
15:O:111:GLU:O	15:O:115:LYS:N	2.13	0.79
21:U:57:GLU:HA	21:U:60:ARG:HB2	1.62	0.79
66:BO:87:ARG:HB3	66:BO:90:HIS:HB3	1.63	0.79
66:BO:86:GLU:HA	66:BO:92:ARG:HH12	1.46	0.79
66:BO:91:CYS:HB3	66:BO:93:VAL:HG22	1.65	0.79
9:I:89:ARG:NH2	71:1:599:U:OP1	2.16	0.79
21:U:37:ASN:ND2	21:U:60:ARG:HG2	1.97	0.79
71:1:158:A:N6	71:1:166:U:OP1	2.15	0.79
9:I:223:HIS:HE1	54:BF:87:LEU:H	1.29	0.78
47:BH:102:SER:O	47:BH:141:GLN:NE2	2.17	0.78
71:1:959:G:O6	71:1:967:A:N6	2.16	0.78
8:H:7:ARG:HB3	8:H:8:PRO:HD2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:143:LEU:HD13	52:BP:171:PHE:HB3	1.64	0.78
44:BM:73:THR:OG1	44:BM:323:ARG:NH2	2.17	0.78
2:B:192:ASP:OD1	2:B:192:ASP:N	2.17	0.78
12:L:2:LEU:N	12:L:14:GLN:OE1	2.17	0.78
71:1:772:U:O2	71:1:1051:A:O2'	2.00	0.78
8:H:101:ARG:HH11	8:H:108:ASN:HD21	1.30	0.78
29:BB:19:VAL:HG12	29:BB:20:HIS:HD2	1.48	0.78
50:BE:56:HIS:HD2	50:BE:57:THR:H	1.28	0.78
65:BL:175:PHE:HB2	65:BL:184:ALA:HB3	1.66	0.77
21:U:29:VAL:HG23	21:U:30:ILE:H	1.48	0.77
71:1:916:U:H4'	71:1:917:A:H5"	1.66	0.77
71:1:1041:U:O4	71:1:1049:A:N6	2.17	0.77
24:X:498:ARG:HG2	24:X:498:ARG:NH1	1.93	0.77
61:BD:49:ARG:NH1	61:BD:57:MET:SD	2.58	0.77
71:1:812:A:H3'	71:1:813:U:H5'	1.67	0.77
19:S:265:HIS:HB2	19:S:268:LYS:HE3	1.67	0.77
71:1:217:A:H62	71:1:323:A:H61	1.32	0.77
9:I:78:ILE:O	9:I:127:LYS:NZ	2.16	0.77
15:O:29:ARG:H	15:O:29:ARG:CD	1.94	0.77
9:I:61:ARG:H	9:I:65:HIS:HD2	1.33	0.77
13:M:97:TRP:O	13:M:97:TRP:CE3	2.38	0.77
26:Z:15:ALA:HB2	26:Z:33:ASP:HB3	1.66	0.77
44:BM:223:ILE:HA	44:BM:228:ASN:HD21	1.50	0.77
65:BL:236:ILE:HG21	65:BL:259:LEU:HD22	1.67	0.77
6:F:113:ARG:HH11	71:1:151:G:H5'	1.49	0.76
7:G:107:ARG:NH1	71:1:182:A:OP2	2.19	0.76
71:1:887:C:O2'	71:1:1083:C:O2	2.02	0.76
1:A:271:ARG:NH2	71:1:815:A:OP2	2.18	0.76
29:BB:122:ASP:OD1	50:BE:56:HIS:ND1	2.19	0.76
71:1:149:U:O2'	71:1:150:A:O5'	2.01	0.76
10:J:77:ASP:HB2	10:J:90:LYS:HB3	1.66	0.76
1:A:383:PHE:CE2	1:A:385:ASP:HB3	2.20	0.76
2:B:229:TYR:OH	2:B:276:ASN:ND2	2.19	0.76
52:BP:59:ARG:NH2	71:1:365:U:OP1	2.18	0.76
71:1:190:A:N6	71:1:207:G:H2'	2.01	0.76
71:1:928:U:O2'	71:1:929:G:OP1	2.01	0.76
24:X:293:ASN:HD21	24:X:348:VAL:HG22	1.50	0.76
1:A:258:ASP:HB2	71:1:1023:A:H5"	1.68	0.76
18:R:455:LYS:HG3	71:1:66:U:H3	1.51	0.76
25:Y:146:ASP:HB3	25:Y:151:ARG:HH22	1.50	0.76
13:M:34:ARG:HH22	71:1:127:A:P	2.09	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:85:ARG:HB2	71:1:313:A:H5"	1.67	0.75
13:M:251:TYR:OH	70:UD:71:UNK:O	2.02	0.75
44:BM:322:TYR:O	44:BM:326:TYR:N	2.19	0.75
71:1:148:U:O2	71:1:149:U:N3	2.18	0.75
19:S:346:SER:HA	19:S:353:ARG:HH21	1.50	0.75
27:BA:85:PRO:HG2	27:BA:87:ILE:HG23	1.67	0.75
71:1:131:U:O2'	71:1:132:U:O5'	2.05	0.75
71:1:384:A:N6	71:1:398:U:O2	2.19	0.75
71:1:163:U:HO2'	71:1:846:A:HO2'	1.32	0.75
21:U:31:PRO:HB3	21:U:60:ARG:HH11	1.50	0.75
66:BO:139:ARG:HH11	66:BO:143:LEU:HD23	1.51	0.75
71:1:642:A:N7	71:1:643:G:N2	2.35	0.74
21:U:32:ARG:HB3	22:V:65:ARG:NH2	2.01	0.74
71:1:699:A:O2'	71:1:700:U:O5'	2.05	0.74
71:1:936:G:N2	71:1:947:U:O2	2.20	0.74
25:Y:245:ASP:OD1	25:Y:246:LYS:N	2.19	0.74
2:B:200:ASN:HB3	2:B:283:LEU:HD22	1.70	0.74
12:L:80:THR:HG22	12:L:120:GLU:HB3	1.70	0.74
29:BB:111:PHE:C	29:BB:111:PHE:HD1	1.90	0.74
44:BM:263:ARG:HG3	44:BM:264:ALA:H	1.50	0.74
22:V:22:ARG:HH21	71:1:314:A:H4'	1.51	0.74
44:BM:76:TYR:O	44:BM:80:ARG:N	2.20	0.74
7:G:13:LEU:O	19:S:309:ARG:NH2	2.21	0.73
13:M:143:TRP:NE1	13:M:206:PRO:HA	2.02	0.73
24:X:267:ASP:HB3	24:X:271:ARG:HA	1.69	0.73
8:H:95:GLN:HA	8:H:109:ILE:HG12	1.71	0.73
47:BH:147:GLY:O	47:BH:149:ASN:ND2	2.20	0.73
54:BF:60:LYS:NZ	71:1:551:A:N7	2.36	0.73
12:L:165:ASP:OD1	12:L:166:TRP:N	2.21	0.73
29:BB:105:GLU:OE1	29:BB:106:PRO:HD2	1.89	0.73
71:1:205:U:O2'	71:1:206:U:H5'	1.88	0.73
61:BD:88:MET:HB3	61:BD:92:GLU:HG3	1.71	0.73
2:B:193:VAL:HG23	2:B:284:LEU:HD12	1.70	0.73
15:O:173:VAL:HA	15:O:192:GLU:HA	1.69	0.73
18:R:398:ASN:HB3	71:1:62:U:C4	2.23	0.73
2:B:82:THR:HG22	2:B:83:VAL:H	1.54	0.73
7:G:10:ARG:NH2	52:BP:-1:GLU:OE2	2.21	0.73
54:BF:14:ARG:NH2	71:1:543:U:OP1	2.20	0.73
66:BO:47:TRP:HD1	71:1:813:U:H5"	1.54	0.73
71:1:755:G:O6	71:1:782:U:O2'	2.06	0.73
9:I:233:ARG:NH1	15:O:97:GLN:OE1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:104:GLN:NE2	71:1:557:A:OP2	2.22	0.73
71:1:841:A:H61	71:1:854:A:H61	1.36	0.73
16:P:51:ARG:O	16:P:53:PHE:N	2.21	0.73
44:BM:68:LEU:HG	44:BM:320:LEU:HA	1.71	0.73
3:C:68:GLU:OE2	3:C:70:ARG:NH1	2.22	0.73
1:A:256:GLY:HA3	66:BO:40:LYS:HG3	1.71	0.72
3:C:96:HIS:HB3	17:Q:79:ASN:HD22	1.50	0.72
8:H:83:THR:HB	8:H:124:GLU:HB2	1.70	0.72
27:BA:131:ARG:NH2	27:BA:138:VAL:O	2.22	0.72
65:BL:147:VAL:HA	65:BL:185:GLU:HG3	1.71	0.72
71:1:533:U:H3	71:1:831:A:H61	1.38	0.72
24:X:374:HIS:ND1	24:X:401:GLU:OE2	2.21	0.72
44:BM:80:ARG:NH2	44:BM:80:ARG:O	2.20	0.72
13:M:205:MET:HB3	13:M:230:HIS:HB2	1.70	0.72
26:Z:48:LYS:HB2	26:Z:80:ARG:HH12	1.53	0.72
44:BM:146:PRO:HB3	44:BM:192:LEU:HD13	1.72	0.72
65:BL:119:ARG:NH1	65:BL:132:HIS:HB3	2.04	0.72
71:1:284:A:H4'	71:1:285:U:OP1	1.88	0.72
71:1:617:G:O2'	71:1:1040:C:OP1	2.08	0.72
71:1:850:U:O2'	71:1:851:U:O5'	2.07	0.72
3:C:177:GLU:HG2	61:BD:58:VAL:H	1.54	0.72
66:BO:175:ASN:HA	66:BO:180:LEU:HD22	1.70	0.72
26:Z:25:PHE:O	26:Z:27:ASP:N	2.22	0.72
20:T:76:GLU:OE2	20:T:79:ARG:NH2	2.21	0.72
24:X:352:LYS:CB	24:X:353:PRO:HD2	2.19	0.71
25:Y:230:ARG:NH1	37:BC:34:GLU:OE1	2.23	0.71
27:BA:113:MET:HG2	27:BA:114:PHE:H	1.55	0.71
71:1:410:A:C8	71:1:490:U:H4'	2.24	0.71
15:O:159:VAL:HG22	15:O:166:ILE:HG12	1.71	0.71
18:R:279:PRO:HA	18:R:282:HIS:HB3	1.73	0.71
23:W:79:HIS:HD2	23:W:88:ARG:HB2	1.53	0.71
65:BL:222:GLU:HB3	65:BL:243:ALA:HB1	1.71	0.71
22:V:63:ARG:NH1	71:1:957:U:OP1	2.23	0.71
44:BM:142:ARG:HH12	44:BM:185:LEU:HD13	1.55	0.71
7:G:373:ARG:HG2	7:G:374:LEU:H	1.54	0.71
50:BE:38:ASP:HB3	50:BE:41:SER:HB3	1.71	0.71
66:BO:82:LYS:HD2	71:1:772:U:C4	2.26	0.71
1:A:392:LEU:HD13	10:J:64:TYR:CD2	2.26	0.71
12:L:71:ARG:O	12:L:73:LEU:N	2.23	0.71
26:Z:104:LYS:HD2	26:Z:108:ARG:HA	1.72	0.71
34:BI:173:GLN:HB3	34:BI:209:GLY:HA3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:202:VAL:HG22	5:E:204:GLY:H	1.54	0.71
11:K:145:HIS:HD2	11:K:147:ALA:H	1.38	0.71
67:BG:1287:CYS:HG	72:BG:1401:ZN:ZN	1.04	0.71
69:UC:66:UNK:O	69:UC:70:UNK:N	2.23	0.70
69:UC:90:UNK:HA	69:UC:94:UNK:HA	1.72	0.70
71:1:433:G:N2	71:1:435:A:H1'	2.06	0.70
71:1:1027:G:N2	71:1:1027:G:OP2	2.24	0.70
1:A:169:ARG:HH21	71:1:1117:U:H3	1.39	0.70
26:Z:81:ARG:NH2	71:1:67:U:OP1	2.24	0.70
47:BH:86:PRO:HA	47:BH:173:VAL:HG22	1.73	0.70
71:1:268:A:H2	71:1:272:A:H1'	1.57	0.70
71:1:320:G:O2'	71:1:377:U:N3	2.23	0.70
1:A:383:PHE:HE2	1:A:385:ASP:HB3	1.55	0.70
5:E:107:TYR:HE2	5:E:113:ILE:HD12	1.57	0.70
65:BL:95:ALA:HA	65:BL:98:MET:HE3	1.72	0.70
67:BG:1287:CYS:SG	72:BG:1401:ZN:ZN	1.81	0.70
71:1:781:A:O2'	71:1:782:U:H2'	1.91	0.70
5:E:206:THR:HG22	5:E:208:LYS:H	1.57	0.70
26:Z:68:ARG:NH2	26:Z:118:HIS:O	2.24	0.70
2:B:384:ARG:NH2	18:R:223:ASP:OD1	2.25	0.70
24:X:172:PRO:HA	24:X:195:GLN:HE21	1.57	0.70
8:H:99:GLU:HG3	71:1:390:A:N3	2.07	0.70
10:J:67:ARG:HB2	10:J:67:ARG:CZ	2.21	0.70
13:M:46:ARG:NH2	71:1:509:U:OP1	2.25	0.70
17:Q:106:THR:HG21	71:1:905:A:N1	2.07	0.70
3:C:142:ASN:ND2	71:1:903:G:OP1	2.24	0.70
7:G:158:SER:O	7:G:161:GLY:N	2.23	0.70
8:H:94:VAL:HB	8:H:108:ASN:HB3	1.74	0.70
22:V:25:VAL:HG22	22:V:26:LEU:H	1.55	0.70
71:1:225:U:H2'	71:1:226:A:H8	1.54	0.70
8:H:72:LEU:O	8:H:77:ARG:NH2	2.25	0.69
21:U:33:LYS:O	21:U:34:ILE:HG13	1.91	0.69
5:E:179:ARG:NH2	71:1:454:A:H1'	2.06	0.69
11:K:81:ARG:NH2	71:1:410:A:OP1	2.25	0.69
26:Z:109:GLY:HA3	71:1:571:U:H4'	1.73	0.69
2:B:290:ASP:HB3	2:B:293:ARG:HE	1.56	0.69
24:X:249:LYS:O	24:X:252:SER:N	2.24	0.69
44:BM:224:PRO:O	44:BM:228:ASN:ND2	2.25	0.69
71:1:159:U:H2'	71:1:160:U:H4'	1.75	0.69
71:1:236:A:H1'	71:1:288:C:H42	1.57	0.69
71:1:1130:A:H61	71:1:1148:A:H62	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:901:G:H22	71:1:908:U:H3	1.38	0.69
65:BL:114:ASP:CB	65:BL:130:LEU:HD13	2.21	0.69
71:1:1074:A:N6	71:1:1086:U:OP2	2.26	0.69
11:K:83:ASP:HB3	11:K:114:CYS:HB2	1.73	0.69
4:D:27:ARG:NE	4:D:29:TYR:OH	2.26	0.69
21:U:30:ILE:HG23	21:U:30:ILE:O	1.92	0.69
44:BM:34:ARG:HD3	44:BM:38:PRO:HG3	1.75	0.69
65:BL:147:VAL:HG13	65:BL:185:GLU:HB2	1.75	0.69
66:BO:172:ARG:HH21	66:BO:172:ARG:CA	2.04	0.69
4:D:135:PRO:HA	4:D:138:VAL:HB	1.73	0.69
5:E:55:PHE:HE2	5:E:104:ILE:HD12	1.58	0.69
7:G:246:GLU:OE2	7:G:295:ARG:NH1	2.26	0.69
29:BB:54:VAL:HG23	29:BB:56:PRO:HD2	1.75	0.69
47:BH:29:VAL:O	47:BH:45:VAL:N	2.23	0.69
71:1:781:A:O2'	71:1:782:U:O5'	2.10	0.69
71:1:1018:A:H62	71:1:1070:C:H42	1.40	0.69
3:C:97:ARG:NH2	61:BD:48:GLN:OE1	2.26	0.69
10:J:54:ILE:HG23	10:J:120:GLY:HA2	1.74	0.69
71:1:983:U:H3'	71:1:984:A:H5"	1.75	0.69
6:F:94:ASP:OD2	29:BB:16:TYR:OH	2.10	0.69
9:I:79:ARG:NH1	54:BF:26:ARG:HE	1.91	0.68
18:R:275:PRO:O	18:R:277:ARG:NH2	2.27	0.68
27:BA:51:ASP:HA	27:BA:54:LYS:HE2	1.75	0.68
44:BM:242:THR:OG1	44:BM:276:HIS:ND1	2.25	0.68
65:BL:128:VAL:HG23	65:BL:128:VAL:O	1.93	0.68
65:BL:320:ASN:ND2	71:1:1087:A:OP2	2.22	0.68
71:1:410:A:H8	71:1:490:U:H4'	1.58	0.68
44:BM:31:ARG:NH1	44:BM:47:LYS:O	2.24	0.68
44:BM:101:LYS:NZ	44:BM:122:LEU:O	2.26	0.68
71:1:336:U:O2	71:1:351:U:O2'	2.09	0.68
7:G:102:GLU:HG2	71:1:183:U:H4'	1.74	0.68
13:M:19:GLN:NE2	71:1:327:U:O2'	2.26	0.68
21:U:41:LEU:HD13	21:U:53:TYR:HB3	1.75	0.68
22:V:120:ALA:HB2	71:1:91:U:H5	1.57	0.68
25:Y:226:LYS:NZ	25:Y:264:GLY:O	2.27	0.68
18:R:236:GLY:O	18:R:237:HIS:ND1	2.24	0.68
29:BB:109:THR:O	29:BB:110:PHE:HB2	1.94	0.68
54:BF:23:PRO:HD2	71:1:595:A:H61	1.57	0.68
2:B:129:LEU:HD12	13:M:7:ARG:HD3	1.75	0.68
14:N:85:ARG:NH2	71:1:314:A:OP2	2.27	0.68
28:UA:71:UNK:O	28:UA:75:UNK:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BL:84:GLN:HE21	65:BL:294:VAL:HG11	1.57	0.68
65:BL:336:PRO:HD2	65:BL:340:VAL:HG13	1.76	0.68
18:R:238:ARG:HH11	18:R:242:ALA:HB1	1.57	0.68
47:BH:188:TRP:CD2	47:BH:227:PRO:HB3	2.29	0.68
70:UD:49:UNK:O	70:UD:53:UNK:N	2.26	0.68
15:O:29:ARG:HD2	15:O:29:ARG:N	2.07	0.68
65:BL:93:VAL:CG1	65:BL:163:VAL:HG22	2.24	0.68
9:I:153:ARG:NH2	71:1:543:U:O4	2.23	0.68
65:BL:251:GLU:OE1	65:BL:372:TRP:N	2.27	0.68
65:BL:305:HIS:HD2	71:1:654:A:H5"	1.59	0.68
8:H:58:MET:HG2	8:H:115:LYS:HG2	1.75	0.68
24:X:247:ALA:HB1	24:X:253:HIS:HB2	1.76	0.68
28:UA:190:UNK:O	28:UA:194:UNK:N	2.27	0.68
71:1:47:A:N6	71:1:130:U:O4	2.26	0.68
29:BB:121:VAL:HG12	50:BE:56:HIS:NE2	2.10	0.67
9:I:84:ILE:HG21	54:BF:12:PHE:HB2	1.76	0.67
26:Z:76:ARG:HH21	26:Z:80:ARG:NH1	1.92	0.67
66:BO:47:TRP:HE3	66:BO:57:GLY:HA2	1.60	0.67
66:BO:172:ARG:HG3	66:BO:172:ARG:O	1.93	0.67
71:1:542:G:O2'	71:1:596:U:O2	2.11	0.67
71:1:638:C:H42	71:1:800:A:H61	1.42	0.67
9:I:61:ARG:NH1	71:1:598:U:OP2	2.27	0.67
9:I:235:TRP:HB3	71:1:596:U:O4	1.94	0.67
16:P:123:ARG:NH2	47:BH:226:GLN:OE1	2.26	0.67
18:R:143:LEU:HD13	18:R:361:VAL:HG13	1.76	0.67
19:S:270:SER:O	19:S:274:ASN:ND2	2.26	0.67
27:BA:23:TYR:O	27:BA:25:ALA:N	2.27	0.67
9:I:42:GLU:HB3	9:I:45:MET:HG3	1.77	0.67
50:BE:56:HIS:HD2	50:BE:57:THR:N	1.93	0.67
34:BI:239:VAL:O	34:BI:243:ILE:N	2.23	0.67
47:BH:123:HIS:O	47:BH:148:ARG:NH1	2.28	0.67
71:1:463:U:N3	71:1:466:U:OP2	2.18	0.67
1:A:283:ARG:HD2	71:1:840:A:H5"	1.77	0.67
47:BH:58:ASN:HD22	47:BH:111:PHE:HE1	1.42	0.67
65:BL:355:GLN:NE2	71:1:664:C:OP2	2.27	0.67
71:1:99:A:H4'	71:1:100:A:H5'	1.76	0.67
71:1:426:G:HO2'	71:1:427:U:P	2.17	0.67
9:I:131:GLU:OE2	9:I:135:ARG:NH1	2.28	0.67
16:P:51:ARG:HD2	16:P:76:THR:HA	1.77	0.67
65:BL:72:ARG:NH2	65:BL:73:SER:OG	2.28	0.67
71:1:433:G:O2'	71:1:434:U:O5'	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BB:17:HIS:ND1	71:1:1118:G:O2'	2.27	0.67
37:BC:59:GLY:O	37:BC:63:ASN:ND2	2.28	0.67
66:BO:117:ARG:NH2	66:BO:119:ARG:O	2.27	0.67
14:N:167:ILE:HG12	14:N:222:VAL:HG22	1.77	0.67
18:R:398:ASN:HB3	71:1:62:U:C5	2.30	0.67
47:BH:79:THR:HG21	47:BH:95:ILE:HD12	1.76	0.67
66:BO:68:CYS:SG	66:BO:76:HIS:ND1	2.67	0.67
71:1:955:U:H5	71:1:970:A:N6	1.92	0.67
25:Y:74:TYR:OH	37:BC:7:ARG:NH2	2.28	0.67
66:BO:103:VAL:HB	66:BO:105:ARG:HB3	1.77	0.67
71:1:1077:G:H22	71:1:1090:U:H3	1.41	0.67
8:H:6:LEU:O	8:H:7:ARG:NH1	2.28	0.66
21:U:25:PHE:HB2	71:1:933:G:N3	2.09	0.66
29:BB:31:ILE:O	29:BB:35:GLU:N	2.27	0.66
71:1:218:A:N6	71:1:319:A:O2'	2.28	0.66
71:1:361:A:H3'	71:1:362:A:H5"	1.75	0.66
71:1:829:U:H2'	71:1:830:A:H8	1.61	0.66
71:1:1018:A:H62	71:1:1070:C:N4	1.93	0.66
6:F:14:TRP:NE1	6:F:50:ASP:OD2	2.26	0.66
18:R:167:HIS:CD2	18:R:169:GLY:H	2.13	0.66
44:BM:76:TYR:OH	44:BM:323:ARG:O	2.13	0.66
61:BD:31:ASN:HD21	61:BD:34:LEU:HG	1.59	0.66
71:1:611:A:H61	71:1:809:A:H5'	1.60	0.66
71:1:890:U:O2	71:1:921:G:N2	2.28	0.66
19:S:355:LYS:NZ	71:1:358:A:OP2	2.25	0.66
71:1:55:A:N6	71:1:122:U:H3	1.92	0.66
7:G:157:VAL:HG21	22:V:58:LEU:HD12	1.77	0.66
10:J:48:HIS:ND1	10:J:48:HIS:O	2.28	0.66
71:1:554:G:C8	71:1:573:A:H2'	2.31	0.66
71:1:639:A:H61	71:1:799:A:H61	1.42	0.66
71:1:975:U:O2	71:1:975:U:C2'	2.40	0.66
2:B:62:TYR:OH	2:B:213:LEU:O	2.13	0.66
2:B:194:LYS:HE2	2:B:194:LYS:O	1.95	0.66
13:M:18:ARG:NH1	71:1:179:U:OP2	2.29	0.66
15:O:263:ASP:O	18:R:41:ARG:NH2	2.28	0.66
25:Y:155:ALA:HA	37:BC:134:GLU:HG2	1.76	0.66
44:BM:218:LEU:O	44:BM:221:ARG:NE	2.29	0.66
65:BL:188:THR:HA	65:BL:278:ARG:O	1.96	0.66
71:1:843:A:H62	71:1:852:A:N6	1.93	0.66
4:D:33:ARG:NH1	4:D:41:CYS:SG	2.68	0.66
22:V:120:ALA:HB2	71:1:91:U:C5	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:864:A:N6	71:1:865:A:N1	2.43	0.66
66:BO:72:THR:HG21	66:BO:162:LEU:HD23	1.75	0.66
1:A:254:ARG:NH2	71:1:1107:A:OP1	2.28	0.66
10:J:57:PRO:HG3	10:J:115:VAL:HG12	1.78	0.66
18:R:272:ARG:HH12	18:R:286:GLN:HE22	1.44	0.66
71:1:39:U:H1'	71:1:40:C:OP1	1.96	0.66
1:A:325:ASP:HA	9:I:28:ASP:HB3	1.77	0.66
6:F:161:GLN:HA	6:F:161:GLN:NE2	2.08	0.66
71:1:204:U:H3'	71:1:204:U:OP2	1.95	0.66
71:1:209:U:P	71:1:209:U:O4'	2.54	0.66
71:1:305:U:OP1	71:1:308:C:N4	2.29	0.66
44:BM:86:LEU:O	44:BM:90:GLN:N	2.29	0.66
65:BL:172:LEU:HB2	65:BL:185:GLU:HB3	1.77	0.66
71:1:663:U:H3	71:1:674:U:H3	1.44	0.66
8:H:40:ASN:OD1	8:H:41:GLU:N	2.29	0.65
16:P:130:VAL:HG12	16:P:132:GLY:H	1.61	0.65
18:R:400:PRO:HB3	71:1:62:U:H5'	1.77	0.65
24:X:498:ARG:HH11	24:X:498:ARG:CG	2.05	0.65
65:BL:141:TRP:CD1	65:BL:141:TRP:O	2.49	0.65
71:1:661:G:H1	71:1:676:U:H3	1.44	0.65
71:1:691:G:N2	71:1:709:U:O2	2.29	0.65
17:Q:50:ASN:OD1	71:1:100:A:O2'	2.14	0.65
1:A:166:HIS:NE2	1:A:220:ALA:O	2.29	0.65
1:A:391:GLN:HG2	66:BO:176:HIS:CE1	2.32	0.65
37:BC:56:LEU:O	37:BC:104:ARG:NH1	2.28	0.65
66:BO:80:ILE:HG22	66:BO:100:ARG:HB3	1.78	0.65
66:BO:172:ARG:CZ	66:BO:172:ARG:HB2	2.27	0.65
1:A:258:ASP:OD1	66:BO:40:LYS:HE2	1.96	0.65
2:B:275:ARG:NH1	2:B:322:THR:O	2.30	0.65
12:L:105:ARG:NH2	71:1:403:U:O2	2.30	0.65
1:A:182:ALA:H	1:A:206:LYS:HB3	1.62	0.65
7:G:131:ASN:ND2	71:1:326:U:O4	2.29	0.65
52:BP:100:ALA:O	52:BP:139:ALA:N	2.29	0.65
66:BO:77:VAL:HB	66:BO:104:GLN:HG3	1.77	0.65
9:I:127:LYS:HB2	9:I:205:MET:HE1	1.79	0.65
16:P:56:ASP:HB3	71:1:952:U:C4	2.32	0.65
18:R:141:VAL:HG11	18:R:345:VAL:HG11	1.79	0.65
65:BL:354:ARG:NH1	71:1:663:U:OP2	2.29	0.65
66:BO:73:ASN:HD22	66:BO:119:ARG:HB3	1.61	0.65
7:G:287:ASN:ND2	71:1:198:A:OP1	2.30	0.65
24:X:348:VAL:HG21	24:X:353:PRO:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:704:U:O2'	71:1:705:A:OP1	2.14	0.65
5:E:52:ASN:N	71:1:467:U:O2'	2.28	0.65
6:F:14:TRP:HB2	6:F:52:VAL:HG12	1.79	0.65
11:K:17:LEU:HD23	11:K:39:ILE:HG23	1.78	0.65
16:P:157:LYS:N	16:P:160:GLU:OE2	2.28	0.65
44:BM:180:LEU:HB2	44:BM:181:PRO:HD3	1.78	0.65
1:A:261:TYR:N	1:A:266:ASP:OD2	2.30	0.65
9:I:185:ARG:HD2	9:I:188:LEU:HD11	1.79	0.65
15:O:292:LEU:HB3	18:R:124:TYR:HB2	1.77	0.65
24:X:367:GLN:HB3	24:X:384:LYS:HE3	1.77	0.65
26:Z:43:ILE:O	26:Z:43:ILE:CG2	2.45	0.65
44:BM:317:PHE:HB2	44:BM:322:TYR:CE1	2.31	0.65
66:BO:174:VAL:O	66:BO:175:ASN:HB2	1.97	0.65
2:B:99:ASN:ND2	2:B:235:THR:O	2.30	0.64
5:E:21:PRO:HB2	5:E:224:GLN:HE22	1.61	0.64
15:O:229:ARG:HD3	15:O:238:LEU:HB3	1.78	0.64
16:P:53:PHE:HB3	16:P:60:ARG:HE	1.62	0.64
18:R:301:PHE:O	18:R:303:ASN:N	2.29	0.64
44:BM:197:PHE:HE2	44:BM:279:TYR:HB3	1.62	0.64
1:A:167:SER:OG	1:A:168:THR:N	2.31	0.64
22:V:104:ARG:NH1	71:1:184:G:O5'	2.30	0.64
24:X:357:THR:O	24:X:361:ARG:NH1	2.30	0.64
27:BA:57:LEU:HA	27:BA:60:ASP:HB2	1.79	0.64
44:BM:141:ARG:NH2	44:BM:268:HIS:O	2.30	0.64
44:BM:141:ARG:NE	44:BM:271:ARG:HB2	2.11	0.64
44:BM:285:LEU:HB3	44:BM:289:ARG:HE	1.61	0.64
66:BO:47:TRP:CD1	71:1:813:U:H5"	2.32	0.64
1:A:138:ALA:HA	10:J:21:PHE:HZ	1.63	0.64
1:A:263:TRP:NE1	71:1:810:U:OP2	2.21	0.64
24:X:301:SER:HA	24:X:306:ALA:HB2	1.78	0.64
26:Z:58:ASP:OD1	26:Z:58:ASP:N	2.30	0.64
44:BM:45:SER:HB2	44:BM:118:ILE:HD13	1.77	0.64
71:1:132:U:H5"	71:1:133:A:H2	1.63	0.64
10:J:87:GLY:HA3	10:J:106:ALA:HB3	1.80	0.64
12:L:70:GLY:HA3	12:L:74:LEU:HG	1.79	0.64
13:M:202:ILE:HD13	13:M:233:LEU:HD13	1.79	0.64
15:O:29:ARG:HG2	15:O:33:ARG:HB2	1.79	0.64
37:BC:29:THR:HG21	37:BC:36:LEU:HB2	1.78	0.64
44:BM:251:ARG:NH1	44:BM:253:CYS:SG	2.63	0.64
44:BM:366:VAL:HB	44:BM:374:LEU:HD13	1.80	0.64
65:BL:241:GLY:O	65:BL:277:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:ASP:HA	3:C:26:PRO:HB3	1.79	0.64
14:N:201:ARG:NH1	14:N:217:ASP:OD2	2.31	0.64
15:O:60:LYS:HD3	15:O:62:GLY:H	1.63	0.64
29:BB:111:PHE:CD1	29:BB:112:LEU:O	2.50	0.64
29:BB:125:LYS:HG3	29:BB:127:PRO:HD3	1.80	0.64
9:I:139:MET:HE1	9:I:166:LYS:HD3	1.80	0.64
24:X:172:PRO:HG2	24:X:220:GLN:HB3	1.78	0.64
29:BB:111:PHE:HE1	29:BB:112:LEU:O	1.81	0.64
71:1:593:U:O2'	71:1:594:U:OP2	2.15	0.64
71:1:639:A:H2'	71:1:640:A:H8	1.62	0.64
17:Q:218:ARG:O	17:Q:218:ARG:NH2	2.29	0.64
18:R:241:SER:O	18:R:245:SER:N	2.30	0.64
26:Z:108:ARG:HE	71:1:571:U:H1'	1.63	0.64
2:B:100:ASN:OD1	2:B:101:VAL:N	2.30	0.64
18:R:73:GLU:OE1	18:R:73:GLU:N	2.30	0.64
24:X:249:LYS:O	24:X:253:HIS:N	2.31	0.64
54:BF:47:ALA:O	54:BF:51:LYS:NZ	2.31	0.64
66:BO:47:TRP:CE3	66:BO:57:GLY:HA2	2.32	0.64
8:H:82:LEU:HD11	8:H:123:PHE:HB3	1.80	0.64
65:BL:167:ARG:HH11	65:BL:299:PRO:HD2	1.62	0.64
69:UC:126:UNK:O	69:UC:130:UNK:N	2.31	0.64
71:1:850:U:O2'	71:1:851:U:O4'	2.16	0.64
71:1:924:U:O2'	71:1:925:G:H8	1.75	0.64
2:B:152:LYS:HG2	2:B:165:GLY:HA3	1.79	0.64
2:B:388:ALA:HB2	18:R:211:SER:HB3	1.80	0.64
25:Y:153:GLN:HE22	37:BC:134:GLU:HB3	1.63	0.63
71:1:870:A:H2'	71:1:871:A:C4	2.32	0.63
2:B:59:PRO:HG2	2:B:88:GLN:HE21	1.63	0.63
6:F:15:LEU:HB2	6:F:140:PRO:HB2	1.80	0.63
22:V:74:LYS:O	22:V:77:ARG:NE	2.31	0.63
26:Z:48:LYS:HB2	26:Z:80:ARG:NH1	2.12	0.63
5:E:300:GLU:OE1	5:E:300:GLU:N	2.31	0.63
13:M:84:GLU:HA	13:M:93:THR:HA	1.79	0.63
66:BO:156:ASN:OD1	66:BO:157:ASP:N	2.30	0.63
71:1:862:A:N6	71:1:1105:G:H22	1.95	0.63
8:H:7:ARG:HB3	8:H:8:PRO:CD	2.28	0.63
15:O:29:ARG:HG2	15:O:33:ARG:HD3	1.79	0.63
16:P:37:GLY:O	16:P:114:ARG:NH2	2.30	0.63
25:Y:247:TYR:OH	25:Y:258:TRP:NE1	2.15	0.63
71:1:1130:A:N6	71:1:1148:A:H62	1.97	0.63
52:BP:97:ARG:HB3	52:BP:97:ARG:CZ	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:365:GLU:HG3	2:B:370:VAL:HG13	1.80	0.63
34:BI:170:GLY:O	34:BI:211:GLN:NE2	2.31	0.63
44:BM:317:PHE:HB3	44:BM:321:LYS:HB2	1.80	0.63
3:C:114:PRO:HD2	3:C:174:ILE:HD13	1.80	0.63
14:N:133:ARG:NH1	71:1:72:U:O4	2.30	0.63
15:O:89:HIS:HD2	15:O:91:LYS:H	1.46	0.63
23:W:79:HIS:CD2	23:W:88:ARG:HB2	2.33	0.63
24:X:332:ALA:HB2	24:X:436:ALA:HB2	1.81	0.63
66:BO:151:THR:OG1	66:BO:152:CYS:N	2.29	0.63
71:1:548:A:H2'	71:1:588:A:H2	1.64	0.63
71:1:753:U:N3	71:1:754:A:N1	2.47	0.63
71:1:990:A:H3'	71:1:991:G:H8	1.64	0.63
1:A:299:GLU:HG3	71:1:1155:A:N3	2.14	0.63
21:U:36:ASN:N	21:U:36:ASN:OD1	2.29	0.63
27:BA:26:LYS:HE2	27:BA:28:TYR:HA	1.81	0.63
71:1:391:A:N7	71:1:393:A:N6	2.47	0.63
8:H:53:THR:HA	8:H:153:THR:HG22	1.81	0.63
14:N:108:LYS:NZ	71:1:63:G:OP2	2.32	0.63
13:M:153:LEU:HA	13:M:156:LEU:HD12	1.79	0.62
9:I:105:LYS:NZ	9:I:139:MET:O	2.29	0.62
10:J:49:THR:HG23	10:J:50:LYS:H	1.62	0.62
21:U:56:THR:O	21:U:60:ARG:N	2.32	0.62
2:B:193:VAL:CG2	2:B:284:LEU:HD12	2.30	0.62
15:O:29:ARG:HB2	15:O:32:THR:OG1	1.99	0.62
18:R:153:ARG:NH1	18:R:156:GLU:OE2	2.23	0.62
21:U:25:PHE:CB	71:1:933:G:N2	2.62	0.62
44:BM:82:LEU:HD11	44:BM:382:LEU:HD21	1.82	0.62
47:BH:176:CYS:SG	47:BH:185:SER:OG	2.55	0.62
71:1:974:U:H4'	71:1:975:U:OP1	1.99	0.62
17:Q:108:ILE:CB	71:1:905:A:H62	2.12	0.62
44:BM:147:ASP:OD2	44:BM:182:ARG:NH2	2.32	0.62
50:BE:37:GLU:HB2	71:1:1144:G:N3	2.14	0.62
66:BO:104:GLN:C	66:BO:105:ARG:HD3	2.19	0.62
71:1:47:A:H4'	71:1:48:U:OP1	2.00	0.62
71:1:53:A:N6	71:1:124:A:H62	1.96	0.62
6:F:114:LYS:HD2	71:1:150:A:H5"	1.80	0.62
9:I:77:LEU:HD13	9:I:83:VAL:HG12	1.81	0.62
27:BA:103:ILE:HG13	27:BA:103:ILE:O	2.00	0.62
65:BL:335:HIS:CD2	65:BL:337:ARG:HH21	2.18	0.62
66:BO:183:VAL:O	66:BO:185:LEU:N	2.25	0.62
14:N:229:VAL:HG12	18:R:10:VAL:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:208:U:H4'	71:1:209:U:OP1	1.96	0.62
71:1:345:A:H62	71:1:379:U:H5'	1.64	0.62
71:1:770:A:N1	71:1:774:A:O2'	2.27	0.62
20:T:80:GLN:HG3	20:T:81:ILE:H	1.63	0.62
21:U:18:LEU:HD23	21:U:19:LYS:H	1.63	0.62
21:U:25:PHE:HB2	71:1:933:G:N2	2.14	0.62
1:A:235:GLN:NE2	1:A:334:ASP:OD1	2.32	0.62
5:E:179:ARG:HH11	5:E:179:ARG:HG3	1.64	0.62
13:M:6:PRO:HB2	13:M:8:TYR:CD2	2.35	0.62
23:W:76:CYS:SG	23:W:89:CYS:HB3	2.40	0.62
50:BE:65:PHE:CZ	50:BE:67:LYS:HE3	2.34	0.62
71:1:1068:A:H4'	71:1:1069:U:H5'	1.82	0.62
9:I:234:TYR:O	71:1:579:U:N3	2.29	0.62
65:BL:98:MET:HG3	65:BL:163:VAL:HG11	1.82	0.62
66:BO:176:HIS:HD2	66:BO:178:TYR:H	1.48	0.62
71:1:1127:U:O2'	71:1:1128:U:OP1	2.16	0.62
8:H:152:GLN:HE22	52:BP:175:MET:HA	1.63	0.62
22:V:47:MET:HE2	24:X:459:ARG:HG3	1.81	0.62
28:UA:162:UNK:O	28:UA:166:UNK:N	2.32	0.62
44:BM:79:ARG:HB3	44:BM:382:LEU:HD13	1.82	0.62
71:1:642:A:O2'	71:1:643:G:OP1	2.14	0.62
1:A:286:PRO:HG2	6:F:77:ALA:O	2.00	0.61
44:BM:17:ARG:NH2	44:BM:19:PHE:O	2.33	0.61
47:BH:72:CYS:HB3	47:BH:96:LEU:HD12	1.82	0.61
47:BH:123:HIS:NE2	47:BH:156:PHE:O	2.33	0.61
52:BP:97:ARG:HB3	52:BP:97:ARG:NH2	2.15	0.61
65:BL:305:HIS:N	71:1:655:U:OP1	2.32	0.61
9:I:194:GLU:HA	9:I:197:LYS:HG2	1.82	0.61
9:I:232:LEU:HD13	54:BF:16:TRP:HB2	1.80	0.61
14:N:72:THR:N	71:1:316:A:OP1	2.28	0.61
14:N:87:PHE:HB2	22:V:19:ARG:NH2	2.14	0.61
34:BI:190:SER:OG	34:BI:224:ASN:O	2.16	0.61
71:1:159:U:N3	71:1:166:U:OP2	2.34	0.61
5:E:186:ARG:HH22	71:1:458:A:N6	1.98	0.61
6:F:115:LEU:HA	6:F:118:ARG:HE	1.65	0.61
11:K:119:ALA:HB2	52:BP:-23:PRO:HB2	1.82	0.61
17:Q:143:ARG:HB3	17:Q:148:LEU:HB2	1.82	0.61
18:R:267:PRO:HG2	18:R:305:THR:HG21	1.82	0.61
27:BA:66:ALA:HB1	27:BA:87:ILE:HA	1.82	0.61
65:BL:335:HIS:HA	65:BL:340:VAL:HG11	1.83	0.61
16:P:112:ARG:HH22	47:BH:219:LYS:HE2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BM:138:VAL:HG23	44:BM:139:PRO:HD3	1.82	0.61
50:BE:54:ALA:O	50:BE:68:LEU:HD23	2.01	0.61
71:1:203:A:H3'	71:1:204:U:H5'	1.81	0.61
71:1:527:U:O2'	71:1:528:A:H8	1.83	0.61
1:A:300:THR:O	71:1:1154:A:O2'	2.18	0.61
15:O:266:THR:HG23	18:R:43:SER:H	1.66	0.61
21:U:29:VAL:HG23	21:U:30:ILE:N	2.15	0.61
24:X:400:VAL:O	24:X:404:ILE:HG12	2.01	0.61
52:BP:97:ARG:N	52:BP:98:PRO:CD	2.57	0.61
65:BL:334:ILE:HB	65:BL:336:PRO:HD3	1.82	0.61
2:B:402:HIS:N	2:B:403:PRO:HD3	2.16	0.61
5:E:186:ARG:HH22	71:1:458:A:H61	1.49	0.61
9:I:180:THR:HG22	20:T:76:GLU:H	1.65	0.61
11:K:44:ARG:NH2	71:1:156:A:OP2	2.28	0.61
18:R:403:LYS:NZ	71:1:63:G:OP1	2.33	0.61
26:Z:43:ILE:O	26:Z:44:LEU:HB3	2.01	0.61
52:BP:182:THR:OG1	52:BP:185:ASP:O	2.17	0.61
8:H:93:VAL:HG12	8:H:94:VAL:HG23	1.81	0.61
14:N:203:ARG:HB2	14:N:215:LEU:HD12	1.81	0.61
27:BA:56:LEU:O	27:BA:60:ASP:N	2.33	0.61
67:BG:1341:VAL:HG23	67:BG:1342:CYS:H	1.64	0.61
15:O:132:LYS:HB2	15:O:133:PRO:HD2	1.83	0.61
47:BH:176:CYS:HG	47:BH:185:SER:HG	1.47	0.61
71:1:865:A:O2'	71:1:870:A:N7	2.29	0.61
9:I:23:ARG:NH2	71:1:600:A:N3	2.48	0.61
9:I:238:ARG:NH2	15:O:88:ARG:O	2.34	0.61
18:R:242:ALA:HA	18:R:245:SER:HB2	1.83	0.61
22:V:61:LYS:HD3	71:1:955:U:H4'	1.83	0.61
71:1:703:U:O2'	71:1:704:U:OP1	2.17	0.61
18:R:126:PRO:O	34:BI:161:GLN:NE2	2.29	0.60
18:R:187:ASP:OD1	18:R:188:ALA:N	2.34	0.60
71:1:650:U:O2'	71:1:651:U:O5'	2.19	0.60
6:F:5:TRP:HE3	6:F:7:CYS:H	1.46	0.60
15:O:157:ILE:HG13	15:O:169:GLN:HB2	1.82	0.60
21:U:25:PHE:HB2	71:1:933:G:C2	2.35	0.60
25:Y:86:ASP:HB2	37:BC:38:LEU:HD21	1.83	0.60
71:1:574:A:O2'	71:1:575:G:O4'	2.19	0.60
71:1:936:G:H1	71:1:947:U:H3	1.49	0.60
71:1:969:U:O2'	71:1:970:A:O4'	2.15	0.60
71:1:1097:A:O2'	71:1:1098:A:OP1	2.16	0.60
11:K:23:MET:SD	71:1:146:U:O4	2.58	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:132:TYR:OH	15:O:71:GLU:OE2	2.18	0.60
17:Q:106:THR:HG21	71:1:905:A:C2	2.37	0.60
25:Y:175:ASP:OD1	25:Y:176:ASP:N	2.34	0.60
71:1:1077:G:N3	71:1:1091:G:N2	2.48	0.60
4:D:102:GLN:O	4:D:106:LEU:N	2.32	0.60
6:F:113:ARG:NH1	71:1:151:G:H5'	2.16	0.60
8:H:72:LEU:HB3	8:H:77:ARG:HH22	1.65	0.60
14:N:138:PHE:O	14:N:142:PHE:N	2.24	0.60
24:X:170:VAL:HG12	24:X:206:THR:HG22	1.82	0.60
25:Y:108:LEU:HB3	25:Y:111:ALA:HB3	1.84	0.60
61:BD:47:GLU:OE1	61:BD:50:ARG:NH1	2.34	0.60
71:1:862:A:H61	71:1:1105:G:H22	1.48	0.60
11:K:14:THR:OG1	71:1:522:U:N3	2.35	0.60
13:M:12:LEU:HD13	13:M:13:ARG:HB2	1.84	0.60
13:M:214:ASP:HB3	13:M:222:ALA:O	2.01	0.60
14:N:194:ARG:HB2	71:1:565:U:H3	1.67	0.60
18:R:40:ARG:HA	18:R:101:ARG:HH21	1.67	0.60
26:Z:56:GLY:HA3	26:Z:61:GLY:HA2	1.83	0.60
44:BM:17:ARG:HH22	44:BM:19:PHE:HB3	1.65	0.60
52:BP:-4:THR:O	52:BP:-2:ILE:N	2.35	0.60
71:1:622:U:O4	71:1:623:A:N6	2.34	0.60
71:1:699:A:N3	71:1:699:A:H2'	2.15	0.60
10:J:92:TYR:OH	10:J:99:ASN:ND2	2.35	0.60
13:M:150:LEU:HD13	13:M:202:ILE:HG13	1.84	0.60
17:Q:89:SER:OG	17:Q:90:ARG:N	2.34	0.60
65:BL:139:ARG:O	65:BL:140:SER:HB3	2.02	0.60
71:1:410:A:O2'	71:1:411:U:OP2	2.16	0.60
18:R:411:LYS:NZ	71:1:116:U:H5'	2.16	0.60
26:Z:131:TRP:HZ2	71:1:567:A:C8	2.20	0.60
28:UA:152:UNK:O	28:UA:156:UNK:N	2.34	0.60
71:1:162:G:H8	71:1:164:U:H1'	1.67	0.60
71:1:438:G:H22	71:1:446:U:H3	1.50	0.60
71:1:841:A:H61	71:1:854:A:N6	2.00	0.60
9:I:18:HIS:HB3	71:1:815:A:O2'	2.02	0.60
17:Q:84:GLU:HB3	17:Q:99:LEU:HD23	1.82	0.60
24:X:240:ALA:HB1	24:X:243:ALA:HB3	1.84	0.60
26:Z:86:ILE:HA	26:Z:89:VAL:HG12	1.82	0.60
44:BM:128:LEU:HB2	44:BM:278:LEU:HD22	1.82	0.60
47:BH:191:ASP:OD1	47:BH:192:CYS:N	2.35	0.60
50:BE:56:HIS:CD2	50:BE:57:THR:H	2.13	0.60
71:1:1038:U:O4	71:1:1055:U:O2'	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:59:ARG:NH2	71:1:601:A:OP2	2.35	0.60
13:M:159:ARG:HE	13:M:243:LEU:HD22	1.66	0.60
71:1:641:A:N6	71:1:795:U:O2'	2.35	0.60
71:1:681:G:H1	71:1:793:C:H42	1.50	0.60
2:B:124:ASN:HB2	2:B:199:SER:CB	2.22	0.60
26:Z:76:ARG:HD3	26:Z:77:GLY:N	2.17	0.60
44:BM:311:CYS:HB3	44:BM:314:GLN:HB2	1.84	0.60
52:BP:63:GLU:HG3	52:BP:65:LEU:HB2	1.84	0.60
71:1:162:G:C8	71:1:164:U:H1'	2.36	0.60
71:1:527:U:O2'	71:1:528:A:OP2	2.17	0.60
22:V:123:LEU:HB2	22:V:126:TRP:HD1	1.67	0.59
66:BO:39:ARG:HG3	66:BO:40:LYS:H	1.67	0.59
71:1:202:A:H4'	71:1:203:A:O4'	2.01	0.59
3:C:216:GLU:OE1	3:C:216:GLU:N	2.35	0.59
6:F:76:THR:HG21	71:1:1120:U:H5"	1.84	0.59
7:G:46:LEU:HD21	19:S:338:PRO:HG2	1.83	0.59
18:R:170:ILE:HD11	18:R:173:LEU:HB3	1.83	0.59
24:X:252:SER:HA	24:X:257:ASN:HB3	1.84	0.59
24:X:359:GLU:HG2	24:X:361:ARG:H	1.66	0.59
24:X:498:ARG:O	24:X:501:THR:HG22	2.03	0.59
71:1:559:U:O2'	71:1:560:U:OP1	2.18	0.59
3:C:72:PRO:HB2	3:C:73:MET:HE2	1.84	0.59
7:G:227:PRO:HG2	7:G:228:TYR:CD2	2.37	0.59
15:O:268:ASP:N	15:O:268:ASP:OD1	2.34	0.59
17:Q:37:MET:HG3	17:Q:39:LEU:HG	1.84	0.59
21:U:20:LYS:O	71:1:970:A:H5'	2.02	0.59
71:1:98:G:H2'	71:1:98:G:N3	2.17	0.59
7:G:145:ARG:H	71:1:347:A:H1'	1.68	0.59
15:O:318:LEU:O	15:O:322:THR:N	2.34	0.59
54:BF:101:LEU:HD21	54:BF:106:ILE:HD13	1.84	0.59
65:BL:153:LYS:HD3	65:BL:272:HIS:CE1	2.37	0.59
65:BL:303:LYS:NZ	71:1:676:U:OP2	2.35	0.59
67:BG:1263:HIS:CB	67:BG:1266:GLY:H	2.15	0.59
71:1:145:A:C3'	71:1:146:U:H5"	2.33	0.59
71:1:269:A:O2'	71:1:270:A:OP1	2.15	0.59
71:1:689:U:O2'	71:1:690:U:OP1	2.17	0.59
16:P:79:LEU:HD12	16:P:101:LEU:HD22	1.83	0.59
65:BL:284:ASN:HD22	71:1:671:U:H1'	1.66	0.59
71:1:1113:G:C6	71:1:1114:A:H2	2.20	0.59
1:A:291:ALA:O	71:1:1106:U:O2'	2.19	0.59
13:M:38:TYR:OH	13:M:46:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:97:TRP:CZ3	13:M:99:LEU:HG	2.38	0.59
13:M:229:SER:OG	13:M:230:HIS:N	2.35	0.59
15:O:131:ILE:HG22	15:O:132:LYS:HG2	1.82	0.59
15:O:139:GLY:N	15:O:156:ILE:O	2.34	0.59
24:X:494:LEU:N	24:X:494:LEU:HD12	2.16	0.59
44:BM:346:LEU:HG	44:BM:348:ARG:H	1.68	0.59
71:1:560:U:OP1	71:1:560:U:H2'	2.03	0.59
7:G:161:GLY:HA2	22:V:42:MET:HA	1.84	0.59
8:H:96:LYS:HB2	71:1:390:A:OP1	2.03	0.59
10:J:125:TYR:OH	10:J:129:ARG:NH2	2.23	0.59
12:L:61:VAL:HG21	12:L:77:VAL:HG21	1.85	0.59
15:O:113:HIS:ND1	71:1:129:U:H1'	2.17	0.59
16:P:33:HIS:HB2	16:P:45:LYS:O	2.02	0.59
16:P:52:ARG:C	16:P:60:ARG:HG2	2.22	0.59
17:Q:76:ILE:HG12	17:Q:150:SER:HB2	1.85	0.59
44:BM:209:ALA:HB1	44:BM:213:ARG:NH1	2.18	0.59
67:BG:1304:MET:HG2	67:BG:1306:GLY:H	1.68	0.59
71:1:827:A:O2'	71:1:828:A:OP2	2.21	0.59
5:E:303:PRO:HB2	5:E:307:ARG:HH12	1.66	0.59
7:G:207:ALA:HB2	71:1:189:U:N3	2.17	0.59
7:G:293:ARG:NE	7:G:374:LEU:OXT	2.35	0.59
10:J:88:GLY:HA2	10:J:103:TRP:CE3	2.37	0.59
25:Y:56:ASP:OD1	25:Y:58:ARG:NH2	2.32	0.59
47:BH:57:GLU:OE2	47:BH:61:SER:OG	2.19	0.59
69:UC:74:UNK:O	69:UC:78:UNK:N	2.36	0.59
71:1:840:A:N1	71:1:855:A:H2	2.01	0.59
71:1:894:U:O2'	71:1:918:A:N6	2.36	0.59
1:A:272:ARG:NH2	71:1:1065:U:O2'	2.35	0.59
5:E:277:LEU:HD13	5:E:336:ALA:HB2	1.82	0.59
15:O:67:ILE:N	71:1:134:A:H61	2.01	0.59
21:U:25:PHE:HB2	71:1:933:G:H21	1.67	0.59
21:U:30:ILE:O	21:U:30:ILE:CG2	2.51	0.59
37:BC:45:MET:O	37:BC:49:ASN:ND2	2.35	0.59
52:BP:157:ARG:NH2	52:BP:169:ASP:OD2	2.35	0.59
71:1:204:U:H3'	71:1:204:U:P	2.43	0.59
71:1:798:A:N3	71:1:798:A:H2'	2.17	0.59
1:A:386:GLU:OE1	10:J:63:GLU:HA	2.03	0.59
4:D:122:PHE:HA	4:D:125:PHE:HB3	1.85	0.59
5:E:69:GLY:HA2	5:E:79:ALA:HB3	1.84	0.59
6:F:87:LEU:HD11	6:F:98:VAL:HG13	1.84	0.59
14:N:198:ARG:HH21	14:N:220:VAL:HG11	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BM:185:LEU:HD23	44:BM:193:ALA:HA	1.85	0.59
65:BL:167:ARG:NH1	65:BL:299:PRO:HD2	2.18	0.59
1:A:283:ARG:O	1:A:284:ILE:C	2.41	0.58
8:H:93:VAL:O	8:H:95:GLN:N	2.23	0.58
17:Q:114:LEU:O	17:Q:116:HIS:N	2.36	0.58
26:Z:50:PRO:HD2	26:Z:53:MET:HE3	1.84	0.58
29:BB:128:ASP:OD1	29:BB:129:THR:N	2.36	0.58
65:BL:82:ILE:H	65:BL:82:ILE:HD12	1.68	0.58
66:BO:73:ASN:HB2	66:BO:119:ARG:HA	1.83	0.58
66:BO:148:ASP:OD1	66:BO:149:ARG:HG2	2.02	0.58
71:1:596:U:H1'	71:1:597:U:OP1	2.03	0.58
71:1:790:U:H4'	71:1:791:U:OP1	2.02	0.58
5:E:81:ASP:OD1	5:E:82:PHE:N	2.35	0.58
5:E:277:LEU:HD12	5:E:333:GLN:HA	1.85	0.58
11:K:132:GLU:OE2	11:K:150:ARG:NE	2.36	0.58
16:P:39:PRO:HA	16:P:86:VAL:HA	1.85	0.58
20:T:72:TRP:NE1	20:T:82:LYS:HB3	2.18	0.58
44:BM:28:VAL:HG22	44:BM:180:LEU:HD22	1.85	0.58
7:G:237:ALA:HB2	7:G:252:PHE:CZ	2.38	0.58
15:O:258:ALA:O	15:O:262:ALA:N	2.37	0.58
21:U:25:PHE:CE1	71:1:950:A:C5	2.92	0.58
29:BB:66:TRP:HD1	29:BB:74:PHE:HZ	1.50	0.58
44:BM:119:THR:O	44:BM:122:LEU:N	2.31	0.58
71:1:315:A:O2'	71:1:317:A:OP2	2.21	0.58
26:Z:19:TYR:HB2	71:1:907:G:N3	2.18	0.58
44:BM:149:ALA:HB1	44:BM:250:GLU:OE2	2.03	0.58
65:BL:360:GLN:O	65:BL:361:THR:HG23	2.02	0.58
2:B:311:PRO:HG2	2:B:314:ARG:HG2	1.85	0.58
7:G:79:TRP:CD2	7:G:90:ILE:HD12	2.38	0.58
10:J:67:ARG:HB2	10:J:67:ARG:HH21	1.68	0.58
16:P:55:GLN:HB3	71:1:949:U:H1'	1.84	0.58
44:BM:132:ALA:HB2	44:BM:278:LEU:HD11	1.85	0.58
44:BM:240:ASP:HB3	44:BM:279:TYR:CD2	2.38	0.58
66:BO:131:PHE:HB2	66:BO:151:THR:HG23	1.86	0.58
3:C:150:PRO:HA	17:Q:110:TYR:CG	2.37	0.58
11:K:62:VAL:HG23	11:K:97:GLN:HB2	1.84	0.58
24:X:46:GLU:HA	24:X:49:ARG:HB3	1.84	0.58
12:L:9:ILE:HG23	12:L:13:LEU:HD13	1.86	0.58
15:O:223:THR:HG22	15:O:225:GLU:HG2	1.85	0.58
19:S:341:PHE:HB2	52:BP:52:ARG:HH22	1.67	0.58
37:BC:68:ASP:N	37:BC:68:ASP:OD1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BM:128:LEU:O	44:BM:132:ALA:N	2.34	0.58
71:1:641:A:H2'	71:1:796:A:H61	1.68	0.58
1:A:162:GLN:HE21	1:A:225:LYS:HG2	1.68	0.58
5:E:184:ALA:HB1	5:E:189:ILE:HB	1.84	0.58
5:E:312:ASN:HB3	5:E:315:LEU:HD13	1.85	0.58
13:M:85:LYS:HD2	13:M:94:GLU:OE2	2.03	0.58
18:R:74:GLU:OE2	18:R:74:GLU:N	2.31	0.58
19:S:327:HIS:CD2	19:S:328:ILE:HG13	2.39	0.58
24:X:124:ASP:N	24:X:124:ASP:OD1	2.35	0.58
29:BB:17:HIS:CG	71:1:1118:G:HO2'	2.21	0.58
47:BH:77:LYS:O	47:BH:228:ARG:NH1	2.36	0.58
71:1:873:U:O4	71:1:1015:A:N6	2.36	0.58
71:1:929:G:H5"	71:1:930:A:C4	2.39	0.58
5:E:42:PRO:HG2	5:E:113:ILE:HG23	1.85	0.58
10:J:99:ASN:N	66:BO:148:ASP:OD2	2.35	0.58
11:K:12:ARG:NH2	71:1:524:U:OP2	2.37	0.58
44:BM:294:ASP:HB3	44:BM:323:ARG:HG3	1.86	0.58
54:BF:22:HIS:HA	71:1:595:A:N6	2.19	0.58
65:BL:109:GLY:O	65:BL:110:PHE:HB2	2.03	0.58
65:BL:316:ALA:HB2	65:BL:326:LEU:HD22	1.85	0.58
71:1:513:U:O2'	71:1:514:U:OP1	2.22	0.58
71:1:1046:G:H21	71:1:1047:C:H41	1.52	0.58
8:H:163:GLU:HA	8:H:166:VAL:HG22	1.85	0.57
9:I:175:LYS:H	9:I:201:ARG:NH1	1.95	0.57
9:I:223:HIS:CE1	54:BF:87:LEU:H	2.17	0.57
14:N:234:LYS:O	18:R:24:ASN:ND2	2.37	0.57
15:O:194:PRO:HD3	18:R:434:LEU:HD13	1.84	0.57
16:P:30:LYS:HG3	16:P:50:ARG:HG2	1.86	0.57
20:T:73:CYS:SG	72:T:101:ZN:ZN	1.84	0.57
29:BB:72:HIS:NE2	50:BE:80:SER:HB3	2.19	0.57
47:BH:96:LEU:HD23	47:BH:97:THR:HG23	1.86	0.57
7:G:80:SER:OG	7:G:83:ASP:OD2	2.21	0.57
10:J:100:MET:HE2	66:BO:147:PHE:CE2	2.39	0.57
11:K:168:LEU:HD13	11:K:175:THR:HB	1.85	0.57
16:P:55:GLN:HG3	71:1:935:G:N3	2.19	0.57
25:Y:122:GLN:HG3	25:Y:123:PRO:HD2	1.86	0.57
47:BH:229:TYR:CE2	52:BP:59:ARG:HD2	2.39	0.57
54:BF:11:SER:O	54:BF:12:PHE:HB3	2.04	0.57
71:1:293:U:N3	71:1:919:U:O2	2.37	0.57
1:A:285:TYR:CG	6:F:79:PRO:HG3	2.40	0.57
18:R:319:ARG:NH2	18:R:325:GLU:OE2	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:108:ASN:HB3	10:J:111:LEU:HB2	1.86	0.57
11:K:25:ARG:HA	71:1:41:A:H5"	1.87	0.57
27:BA:42:SER:HB2	27:BA:139:THR:HA	1.85	0.57
44:BM:251:ARG:HH21	44:BM:263:ARG:NH2	2.03	0.57
71:1:433:G:C2	71:1:435:A:H1'	2.38	0.57
7:G:190:ASN:HB3	7:G:193:GLU:HG2	1.86	0.57
19:S:270:SER:OG	19:S:271:TRP:N	2.38	0.57
26:Z:55:HIS:HA	26:Z:64:ILE:HD11	1.86	0.57
71:1:331:U:O2	71:1:502:U:H5'	2.04	0.57
5:E:134:GLY:HA2	71:1:437:U:H5"	1.87	0.57
9:I:215:LYS:HB3	54:BF:28:GLY:HA3	1.86	0.57
11:K:14:THR:O	11:K:18:ASP:N	2.32	0.57
17:Q:62:PRO:O	71:1:81:U:O2'	2.18	0.57
24:X:349:PRO:HD2	24:X:398:ARG:HB3	1.86	0.57
44:BM:28:VAL:HG12	44:BM:30:GLU:H	1.68	0.57
44:BM:263:ARG:HG3	44:BM:264:ALA:N	2.18	0.57
54:BF:9:TYR:OH	71:1:543:U:OP2	2.21	0.57
65:BL:106:ASP:OD1	65:BL:107:TRP:N	2.38	0.57
71:1:110:U:O2'	71:1:111:A:OP1	2.21	0.57
71:1:141:A:H2	71:1:858:A:H62	1.51	0.57
5:E:21:PRO:HB2	5:E:224:GLN:NE2	2.19	0.57
7:G:156:ARG:NH2	7:G:159:ALA:O	2.38	0.57
11:K:123:PRO:HB3	52:BP:3:HIS:O	2.04	0.57
12:L:53:ILE:O	12:L:81:ALA:N	2.33	0.57
15:O:169:GLN:HA	15:O:192:GLU:HG2	1.87	0.57
22:V:32:PHE:HB2	22:V:98:LYS:HE3	1.86	0.57
29:BB:11:SER:HA	71:1:857:A:H5"	1.85	0.57
29:BB:61:TYR:OH	29:BB:65:ARG:NH2	2.36	0.57
67:BG:1325:TRP:CZ2	67:BG:1329:ARG:HD2	2.40	0.57
69:UC:130:UNK:O	69:UC:134:UNK:N	2.38	0.57
71:1:267:U:O2	71:1:269:A:N6	2.38	0.57
71:1:268:A:C2	71:1:272:A:H1'	2.39	0.57
71:1:322:A:N7	71:1:990:A:O2'	2.37	0.57
71:1:445:A:N7	71:1:461:U:H5	2.03	0.57
2:B:15:ARG:NE	13:M:99:LEU:HD11	2.20	0.57
7:G:164:ASN:HA	22:V:111:ARG:NH2	2.20	0.57
11:K:36:LEU:O	11:K:40:THR:HG22	2.05	0.57
15:O:218:VAL:HG11	15:O:229:ARG:HE	1.69	0.57
24:X:165:VAL:HG21	24:X:341:LEU:HD23	1.85	0.57
44:BM:244:LEU:HD12	44:BM:247:PHE:HB3	1.87	0.57
65:BL:246:VAL:HA	65:BL:257:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:ASP:OD1	2:B:11:ASP:N	2.32	0.57
10:J:65:ASN:O	10:J:67:ARG:N	2.38	0.57
13:M:99:LEU:HD23	13:M:108:GLN:HA	1.87	0.57
22:V:79:TYR:HD2	24:X:477:TRP:HE3	1.52	0.57
24:X:293:ASN:ND2	24:X:348:VAL:HG22	2.19	0.57
71:1:508:G:O2'	71:1:509:U:OP1	2.23	0.57
9:I:148:ARG:HH22	9:I:152:ARG:HE	1.53	0.57
18:R:38:SER:HA	18:R:41:ARG:HD2	1.87	0.57
24:X:349:PRO:HB2	24:X:352:LYS:HG2	1.87	0.57
66:BO:87:ARG:HH11	66:BO:89:ALA:HB3	1.69	0.57
71:1:364:U:H5'	71:1:365:U:O5'	2.04	0.57
71:1:664:C:H2'	71:1:670:A:N6	2.20	0.57
9:I:25:ALA:O	9:I:52:ARG:NH2	2.37	0.56
9:I:55:LEU:HD23	9:I:55:LEU:H	1.69	0.56
10:J:65:ASN:HB3	66:BO:172:ARG:HD2	1.86	0.56
10:J:82:GLU:HG3	10:J:83:THR:H	1.70	0.56
12:L:93:VAL:HG21	12:L:106:TRP:CE2	2.40	0.56
16:P:62:PRO:HD3	16:P:77:PHE:HE2	1.69	0.56
18:R:284:LYS:HG3	18:R:285:TYR:N	2.20	0.56
21:U:18:LEU:HD23	21:U:19:LYS:N	2.20	0.56
21:U:41:LEU:HB3	21:U:83:MET:HB3	1.87	0.56
26:Z:77:GLY:O	26:Z:80:ARG:NH2	2.37	0.56
29:BB:72:HIS:CE1	50:BE:80:SER:HB3	2.40	0.56
54:BF:22:HIS:O	54:BF:26:ARG:NH1	2.37	0.56
66:BO:80:ILE:HG21	66:BO:100:ARG:NH1	2.19	0.56
66:BO:133:ARG:NH2	66:BO:135:GLN:OE1	2.32	0.56
18:R:119:LYS:HB3	18:R:121:ILE:HG23	1.87	0.56
71:1:381:A:O2'	71:1:382:A:OP1	2.20	0.56
71:1:478:A:H4'	71:1:480:A:C6	2.40	0.56
71:1:812:A:H5'	71:1:813:U:OP2	2.04	0.56
71:1:963:A:O2'	71:1:964:A:N3	2.37	0.56
1:A:110:ASP:N	1:A:110:ASP:OD1	2.36	0.56
3:C:52:TRP:HB3	18:R:189:GLU:HG2	1.87	0.56
13:M:46:ARG:HB2	71:1:519:U:H5'	1.86	0.56
13:M:84:GLU:HB3	13:M:93:THR:HG22	1.88	0.56
15:O:230:ARG:NH2	15:O:240:PRO:O	2.33	0.56
23:W:63:LEU:HD13	23:W:98:GLN:HB3	1.86	0.56
25:Y:65:ASP:HA	25:Y:68:ARG:HB2	1.86	0.56
27:BA:67:LEU:O	27:BA:113:MET:HB2	2.05	0.56
29:BB:120:VAL:HG22	29:BB:121:VAL:H	1.70	0.56
34:BI:173:GLN:OE1	34:BI:209:GLY:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BM:35:GLN:HE22	44:BM:44:ALA:HA	1.70	0.56
47:BH:221:VAL:HG22	47:BH:225:ILE:HD11	1.86	0.56
52:BP:97:ARG:NH2	52:BP:97:ARG:CB	2.68	0.56
61:BD:55:SER:OG	61:BD:56:GLY:N	2.39	0.56
65:BL:218:THR:H	65:BL:221:LYS:HZ1	1.53	0.56
66:BO:50:GLY:HA2	66:BO:56:ALA:HB1	1.86	0.56
66:BO:130:LEU:O	66:BO:173:HIS:HE1	1.89	0.56
9:I:171:SER:OG	9:I:172:ASP:N	2.38	0.56
13:M:148:ILE:HG22	15:O:33:ARG:NH1	2.21	0.56
14:N:175:SER:OG	14:N:178:GLU:OE2	2.24	0.56
18:R:112:ILE:O	18:R:115:GLU:HG3	2.05	0.56
19:S:331:ARG:HD3	52:BP:59:ARG:HB2	1.86	0.56
21:U:28:LYS:O	21:U:29:VAL:HG22	2.04	0.56
26:Z:78:ASN:O	26:Z:88:ARG:NH2	2.37	0.56
71:1:639:A:H2'	71:1:640:A:C8	2.40	0.56
71:1:829:U:H2'	71:1:830:A:C8	2.40	0.56
71:1:863:A:C6	71:1:1105:G:N2	2.73	0.56
71:1:1077:G:N2	71:1:1090:U:H3	2.04	0.56
1:A:238:THR:OG1	1:A:302:ASP:O	2.19	0.56
8:H:96:LYS:HD2	8:H:99:GLU:OE1	2.05	0.56
14:N:151:VAL:HG22	14:N:170:ILE:HG22	1.88	0.56
15:O:146:SER:OG	15:O:147:GLY:N	2.38	0.56
22:V:69:ARG:NH1	71:1:953:U:O2'	2.38	0.56
44:BM:188:LYS:O	44:BM:191:GLU:HG2	2.05	0.56
47:BH:68:GLY:HA2	47:BH:214:HIS:HE1	1.70	0.56
50:BE:56:HIS:CD2	50:BE:57:THR:N	2.71	0.56
66:BO:74:CYS:SG	66:BO:76:HIS:HB3	2.46	0.56
66:BO:172:ARG:HA	66:BO:172:ARG:NH2	2.13	0.56
71:1:1017:U:H5"	71:1:1018:A:OP2	2.06	0.56
3:C:102:ILE:O	17:Q:85:ARG:HD2	2.05	0.56
7:G:158:SER:O	7:G:160:GLY:N	2.38	0.56
8:H:61:GLN:NE2	8:H:114:TYR:OH	2.38	0.56
11:K:11:TYR:CZ	11:K:13:ALA:HA	2.40	0.56
22:V:96:ARG:NH2	71:1:374:U:H5'	2.20	0.56
25:Y:204:ARG:NH2	25:Y:218:GLU:OE2	2.37	0.56
44:BM:294:ASP:HB2	44:BM:295:PRO:HD3	1.88	0.56
65:BL:337:ARG:O	71:1:662:G:O2'	2.14	0.56
71:1:391:A:H1'	71:1:392:A:C8	2.40	0.56
71:1:644:C:O2'	71:1:645:G:OP2	2.21	0.56
71:1:1075:A:P	71:1:1075:A:H3'	2.46	0.56
1:A:124:ASN:HB3	1:A:127:TYR:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:SER:OG	2:B:255:ARG:N	2.39	0.56
3:C:140:ASN:OD1	3:C:141:ARG:N	2.39	0.56
10:J:59:THR:O	10:J:70:ARG:HA	2.05	0.56
13:M:68:ARG:NH1	71:1:123:U:OP2	2.39	0.56
17:Q:111:SER:HB3	17:Q:136:PHE:HD2	1.71	0.56
44:BM:76:TYR:HE2	44:BM:323:ARG:HG2	1.71	0.56
65:BL:152:GLN:HB2	65:BL:177:TYR:CE1	2.41	0.56
65:BL:219:TYR:HB2	65:BL:248:ARG:HB2	1.88	0.56
65:BL:264:VAL:HG23	65:BL:351:LEU:HB3	1.87	0.56
71:1:176:A:N6	71:1:526:U:O4	2.23	0.56
3:C:179:PRO:HG3	3:C:185:TYR:CD1	2.41	0.56
7:G:116:GLY:H	71:1:353:A:H4'	1.71	0.56
7:G:201:ARG:NH1	7:G:266:LEU:O	2.39	0.56
15:O:274:PRO:HA	15:O:277:VAL:HG12	1.88	0.56
18:R:414:LEU:HA	18:R:417:VAL:HG12	1.87	0.56
67:BG:1319:SER:HB3	67:BG:1321:ALA:H	1.71	0.56
71:1:177:G:H22	71:1:525:U:H3	1.54	0.56
15:O:213:LEU:HD11	15:O:230:ARG:HB3	1.86	0.56
44:BM:144:LEU:HD21	44:BM:263:ARG:HH22	1.71	0.56
44:BM:177:ARG:NE	44:BM:212:GLU:OE2	2.34	0.56
66:BO:172:ARG:CA	66:BO:172:ARG:NH2	2.69	0.56
3:C:23:THR:HG21	3:C:63:ARG:HG2	1.88	0.56
8:H:99:GLU:HA	71:1:390:A:C5	2.41	0.56
11:K:31:GLU:HB2	11:K:34:VAL:HG12	1.88	0.56
12:L:32:TYR:CZ	12:L:42:VAL:HG12	2.41	0.56
15:O:265:GLU:HA	18:R:41:ARG:HB3	1.88	0.56
21:U:25:PHE:CD2	21:U:25:PHE:O	2.58	0.56
25:Y:44:ALA:HB1	37:BC:99:ILE:HD13	1.88	0.56
28:UA:193:UNK:O	28:UA:197:UNK:N	2.39	0.56
52:BP:-41:ARG:NH2	52:BP:18:GLU:OE2	2.37	0.56
52:BP:-4:THR:O	52:BP:-4:THR:OG1	2.17	0.56
71:1:553:A:H2'	71:1:554:G:H5'	1.88	0.56
8:H:11:LEU:HD12	8:H:14:ALA:N	2.21	0.55
61:BD:8:LYS:HA	61:BD:23:ALA:HA	1.88	0.55
71:1:319:A:O2'	71:1:320:G:OP1	2.22	0.55
71:1:754:A:N6	71:1:784:A:H61	2.03	0.55
5:E:171:PRO:HD2	5:E:176:ARG:NH1	2.21	0.55
12:L:54:ALA:HA	12:L:80:THR:HA	1.89	0.55
13:M:148:ILE:HG22	15:O:33:ARG:CZ	2.35	0.55
19:S:347:VAL:HG12	19:S:348:ALA:H	1.72	0.55
26:Z:54:ASP:O	26:Z:55:HIS:ND1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:112:GLU:OE1	27:BA:112:GLU:N	2.39	0.55
52:BP:95:PRO:O	52:BP:97:ARG:N	2.40	0.55
71:1:303:U:O2'	71:1:304:G:OP1	2.23	0.55
71:1:558:C:N4	71:1:559:U:O4	2.40	0.55
2:B:126:SER:HG	13:M:7:ARG:HH21	1.55	0.55
2:B:295:SER:OG	22:V:28:PRO:HA	2.06	0.55
6:F:114:LYS:NZ	71:1:151:G:OP2	2.29	0.55
11:K:116:SER:OG	12:L:133:LYS:O	2.14	0.55
13:M:110:ASN:OD1	13:M:111:TRP:N	2.39	0.55
24:X:302:THR:H	24:X:306:ALA:N	2.03	0.55
28:UA:90:UNK:O	28:UA:94:UNK:N	2.38	0.55
37:BC:51:ARG:NH2	37:BC:90:GLN:O	2.39	0.55
44:BM:90:GLN:HG2	44:BM:282:ARG:HH21	1.70	0.55
66:BO:92:ARG:NH1	66:BO:97:VAL:HG11	2.22	0.55
3:C:124:GLU:O	3:C:124:GLU:HG2	2.07	0.55
7:G:16:PRO:HG2	7:G:19:GLN:HG2	1.87	0.55
10:J:64:TYR:CG	10:J:64:TYR:O	2.59	0.55
15:O:316:ASP:HA	15:O:319:VAL:HG22	1.88	0.55
17:Q:220:MET:O	17:Q:224:LYS:N	2.38	0.55
25:Y:238:HIS:O	25:Y:244:ARG:NH2	2.40	0.55
44:BM:134:LYS:HG2	44:BM:271:ARG:CZ	2.36	0.55
44:BM:224:PRO:HD2	44:BM:228:ASN:OD1	2.07	0.55
71:1:1075:A:H8	71:1:1075:A:OP2	1.89	0.55
10:J:119:LYS:O	10:J:121:SER:N	2.38	0.55
18:R:278:ASN:O	18:R:282:HIS:N	2.38	0.55
20:T:50:ARG:NH2	71:1:536:A:O2'	2.39	0.55
24:X:349:PRO:HG2	24:X:398:ARG:HG3	1.87	0.55
26:Z:20:PRO:HD3	71:1:907:G:C2	2.42	0.55
65:BL:253:ASN:OD1	65:BL:269:ASN:ND2	2.18	0.55
8:H:42:VAL:HB	8:H:161:VAL:HG13	1.88	0.55
12:L:93:VAL:HG21	12:L:106:TRP:CD2	2.41	0.55
15:O:116:ILE:O	15:O:120:GLY:N	2.35	0.55
22:V:15:GLU:HA	22:V:18:THR:HG22	1.87	0.55
29:BB:124:ALA:HA	50:BE:55:PRO:HD2	1.88	0.55
2:B:177:HIS:HE1	71:1:178:U:OP1	1.90	0.55
5:E:170:TYR:HB3	5:E:171:PRO:HD3	1.88	0.55
8:H:31:LYS:HB2	71:1:388:U:OP2	2.06	0.55
12:L:133:LYS:HB2	12:L:149:ASN:ND2	2.22	0.55
14:N:76:TYR:O	14:N:78:ARG:N	2.39	0.55
14:N:209:VAL:HG11	18:R:419:GLN:HG2	1.89	0.55
18:R:205:TYR:O	18:R:213:THR:OG1	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:289:SER:O	18:R:292:SER:N	2.39	0.55
44:BM:75:VAL:HG12	44:BM:79:ARG:HE	1.72	0.55
52:BP:-16:SER:OG	52:BP:-1:GLU:OE1	2.19	0.55
61:BD:92:GLU:OE1	61:BD:96:ARG:NH1	2.39	0.55
67:BG:1262:CYS:HA	67:BG:1267:ASP:HA	1.89	0.55
67:BG:1278:ARG:HH21	71:1:593:U:H1'	1.72	0.55
71:1:698:G:O6	71:1:699:A:N6	2.39	0.55
6:F:5:TRP:HA	6:F:8:ARG:CZ	2.37	0.55
6:F:62:MET:HB3	6:F:67:TRP:CE2	2.42	0.55
14:N:176:LYS:NZ	71:1:564:U:O4	2.35	0.55
15:O:134:TRP:NE1	15:O:136:TRP:O	2.40	0.55
15:O:173:VAL:HG22	15:O:190:GLN:HB3	1.88	0.55
16:P:88:THR:HG23	16:P:102:ASP:HB2	1.87	0.55
18:R:33:ALA:HB1	18:R:90:SER:HB2	1.88	0.55
22:V:126:TRP:CH2	71:1:90:A:H8	2.24	0.55
24:X:373:LEU:HB3	24:X:374:HIS:HD2	1.72	0.55
26:Z:70:HIS:HB2	26:Z:138:VAL:HG23	1.88	0.55
34:BI:173:GLN:NE2	34:BI:201:ALA:O	2.40	0.55
37:BC:69:THR:OG1	37:BC:72:THR:HG23	2.07	0.55
54:BF:70:ARG:HH21	54:BF:76:SER:CB	2.20	0.55
66:BO:172:ARG:HB2	66:BO:172:ARG:NH2	2.22	0.55
71:1:146:U:O2	71:1:146:U:O4'	2.20	0.55
71:1:711:A:H2'	71:1:711:A:N3	2.22	0.55
71:1:1097:A:HO2'	71:1:1098:A:P	2.29	0.55
3:C:145:ARG:HH12	17:Q:108:ILE:CG2	2.20	0.55
26:Z:131:TRP:CZ2	71:1:567:A:C8	2.95	0.55
34:BI:158:TYR:OH	34:BI:222:HIS:NE2	2.39	0.55
65:BL:127:LYS:O	71:1:667:A:H3'	2.07	0.55
3:C:71:TYR:HB3	3:C:72:PRO:HD3	1.89	0.55
6:F:161:GLN:HE21	6:F:161:GLN:CA	2.15	0.55
18:R:187:ASP:O	18:R:190:GLN:N	2.40	0.55
22:V:66:ARG:HH11	22:V:77:ARG:HH12	1.55	0.55
26:Z:18:VAL:CG2	26:Z:21:PHE:HB2	2.37	0.55
44:BM:118:ILE:HG13	44:BM:119:THR:N	2.21	0.55
52:BP:163:ARG:NE	71:1:473:U:O3'	2.39	0.55
71:1:322:A:N6	71:1:990:A:O2'	2.35	0.55
12:L:44:ARG:NH1	71:1:496:U:OP1	2.40	0.54
18:R:455:LYS:HB3	71:1:66:U:O2	2.06	0.54
21:U:38:MET:O	21:U:38:MET:HG3	2.07	0.54
24:X:404:ILE:HG22	24:X:405:PRO:O	2.07	0.54
24:X:494:LEU:HB2	24:X:496:TRP:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:76:ARG:NH1	71:1:71:A:N3	2.55	0.54
44:BM:318:PRO:HA	44:BM:322:TYR:CD2	2.41	0.54
66:BO:100:ARG:HD2	71:1:772:U:O5'	2.06	0.54
3:C:80:GLU:OE2	3:C:96:HIS:NE2	2.40	0.54
11:K:42:LEU:O	11:K:46:GLN:HG3	2.08	0.54
13:M:94:GLU:OE1	71:1:515:A:N6	2.40	0.54
18:R:84:LEU:HA	18:R:87:VAL:HG12	1.88	0.54
71:1:233:G:H5'	71:1:234:U:OP2	2.07	0.54
71:1:398:U:O2'	71:1:399:U:O5'	2.17	0.54
71:1:1046:G:OP1	71:1:1046:G:H4'	2.06	0.54
2:B:174:TRP:HA	22:V:12:ALA:O	2.08	0.54
2:B:193:VAL:HG23	2:B:284:LEU:CD1	2.37	0.54
3:C:143:VAL:HG12	3:C:148:LEU:HG	1.89	0.54
5:E:281:ASP:HB3	5:E:284:ASP:HB3	1.89	0.54
5:E:303:PRO:HB2	5:E:307:ARG:NH1	2.22	0.54
7:G:58:ASP:OD1	7:G:59:ALA:N	2.40	0.54
10:J:142:ARG:NH1	71:1:806:A:OP2	2.40	0.54
14:N:77:ASN:ND2	71:1:87:A:N3	2.56	0.54
50:BE:92:GLU:HB3	50:BE:95:ARG:HG3	1.88	0.54
71:1:361:A:H3'	71:1:362:A:C5'	2.36	0.54
71:1:561:U:O2'	71:1:562:U:O4'	2.19	0.54
71:1:876:G:C2	71:1:877:G:C4	2.96	0.54
2:B:296:SER:OG	71:1:89:U:H4'	2.08	0.54
4:D:130:LYS:O	4:D:134:LEU:HG	2.07	0.54
7:G:128:ARG:HG2	71:1:320:G:O6	2.07	0.54
7:G:148:THR:O	7:G:148:THR:HG22	2.08	0.54
7:G:349:GLN:HB2	7:G:352:SER:HB3	1.90	0.54
14:N:85:ARG:HH21	71:1:313:A:H3'	1.72	0.54
15:O:320:ARG:O	15:O:323:GLU:HG3	2.06	0.54
26:Z:97:VAL:HB	26:Z:105:LEU:HB2	1.90	0.54
71:1:848:U:H4'	71:1:996:G:OP1	2.07	0.54
9:I:16:MET:HB2	66:BO:46:ARG:HD2	1.88	0.54
9:I:48:TYR:HB3	9:I:57:LYS:HB3	1.89	0.54
10:J:88:GLY:HA2	10:J:103:TRP:HE3	1.71	0.54
10:J:142:ARG:NH2	71:1:615:U:OP2	2.40	0.54
12:L:78:ARG:NH2	52:BP:25:ALA:O	2.41	0.54
19:S:295:PRO:HG2	19:S:296:PRO:HD3	1.89	0.54
22:V:41:GLN:O	22:V:111:ARG:NH1	2.41	0.54
24:X:91:THR:HG22	24:X:94:LEU:HG	1.88	0.54
24:X:216:THR:HA	24:X:421:GLN:NE2	2.22	0.54
25:Y:275:ASP:N	25:Y:275:ASP:OD1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:576:A:H5'	71:1:577:A:H5"	1.88	0.54
71:1:1028:U:O4	71:1:1057:A:N6	2.40	0.54
7:G:255:VAL:HA	7:G:297:TRP:CD1	2.43	0.54
10:J:96:GLU:HG3	10:J:97:GLU:H	1.73	0.54
11:K:25:ARG:HE	71:1:145:A:P	2.31	0.54
11:K:62:VAL:O	11:K:66:VAL:HG12	2.07	0.54
13:M:71:TRP:HA	13:M:76:ASN:ND2	2.23	0.54
13:M:99:LEU:HB3	13:M:106:MET:HE3	1.90	0.54
14:N:77:ASN:ND2	71:1:87:A:H1'	2.22	0.54
15:O:21:TYR:CE1	15:O:28:ALA:HA	2.43	0.54
29:BB:125:LYS:C	29:BB:127:PRO:HD3	2.28	0.54
44:BM:206:GLY:HA3	44:BM:314:GLN:HE21	1.71	0.54
71:1:56:U:O4	71:1:57:A:N6	2.41	0.54
5:E:206:THR:HB	5:E:209:GLN:HG2	1.88	0.54
6:F:12:ARG:HH21	6:F:14:TRP:HZ2	1.53	0.54
7:G:217:VAL:HG23	7:G:236:ASN:O	2.08	0.54
13:M:138:ALA:H	13:M:230:HIS:HD2	1.55	0.54
15:O:114:GLN:O	15:O:118:ILE:HG12	2.08	0.54
19:S:351:HIS:HD2	71:1:358:A:H62	1.56	0.54
26:Z:110:GLY:HA2	71:1:555:U:H3	1.73	0.54
71:1:187:U:H5"	71:1:188:A:H2'	1.90	0.54
71:1:442:U:H4'	71:1:443:G:C8	2.42	0.54
5:E:302:THR:HB	5:E:303:PRO:HD2	1.89	0.54
7:G:189:LEU:HD13	7:G:195:ILE:HG21	1.88	0.54
7:G:207:ALA:N	7:G:210:GLU:OE2	2.41	0.54
11:K:169:GLN:OE1	11:K:174:ARG:NH2	2.41	0.54
13:M:31:HIS:O	22:V:11:LYS:NZ	2.41	0.54
23:W:104:GLU:O	23:W:107:TRP:HD1	1.90	0.54
24:X:126:ARG:HD2	24:X:206:THR:HG21	1.89	0.54
24:X:252:SER:HA	24:X:257:ASN:CB	2.38	0.54
24:X:302:THR:HG22	24:X:304:ASP:H	1.73	0.54
54:BF:33:ASP:N	54:BF:33:ASP:OD1	2.40	0.54
6:F:84:ARG:NH2	23:W:108:THR:OG1	2.41	0.54
7:G:180:LEU:O	7:G:184:VAL:HG23	2.08	0.54
9:I:229:HIS:ND1	9:I:246:VAL:HG11	2.23	0.54
10:J:5:ARG:HD3	71:1:1157:A:C4	2.42	0.54
15:O:20:THR:HG23	15:O:21:TYR:H	1.73	0.54
16:P:112:ARG:HH12	47:BH:219:LYS:HG2	1.73	0.54
17:Q:108:ILE:O	17:Q:108:ILE:CG2	2.48	0.54
19:S:346:SER:HA	19:S:353:ARG:NH2	2.20	0.54
65:BL:167:ARG:NE	65:BL:297:ASN:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:798:A:H2	71:1:799:A:N6	2.04	0.54
9:I:72:ARG:HA	9:I:75:THR:HG22	1.90	0.54
10:J:54:ILE:HD12	10:J:55:GLY:H	1.72	0.54
11:K:23:MET:HG3	71:1:145:A:H2	1.72	0.54
11:K:27:ARG:NH1	71:1:835:A:OP2	2.41	0.54
22:V:138:LEU:HD23	22:V:138:LEU:H	1.72	0.54
25:Y:279:HIS:HB3	25:Y:282:GLN:HE21	1.72	0.54
26:Z:131:TRP:HH2	71:1:566:G:HO2'	1.56	0.54
27:BA:20:GLY:N	52:BP:-10:ARG:HG2	2.22	0.54
47:BH:186:ARG:HB3	47:BH:188:TRP:HZ3	1.73	0.54
65:BL:301:ARG:HH22	71:1:235:G:H4'	1.73	0.54
71:1:163:U:H2'	71:1:166:U:N3	2.23	0.54
71:1:798:A:O2'	71:1:799:A:O5'	2.26	0.54
9:I:115:LEU:HG	9:I:125:VAL:HG12	1.89	0.53
9:I:178:ASP:OD1	9:I:180:THR:HG23	2.08	0.53
10:J:7:ARG:HB3	71:1:1108:A:OP1	2.09	0.53
10:J:111:LEU:HD21	66:BO:143:LEU:HB2	1.88	0.53
24:X:137:TRP:O	24:X:141:ARG:N	2.40	0.53
26:Z:76:ARG:HH11	71:1:71:A:P	2.31	0.53
44:BM:46:ARG:HD2	44:BM:50:LYS:HZ2	1.74	0.53
44:BM:246:ARG:HE	44:BM:269:VAL:N	2.06	0.53
65:BL:336:PRO:HG2	65:BL:339:CYS:HB3	1.89	0.53
66:BO:47:TRP:N	71:1:814:A:H2	2.06	0.53
9:I:66:ARG:NH2	71:1:819:U:OP1	2.40	0.53
12:L:3:ARG:HB2	12:L:126:THR:HG23	1.90	0.53
15:O:184:ARG:HH22	15:O:187:GLN:HG2	1.71	0.53
24:X:265:SER:HB2	24:X:337:HIS:ND1	2.23	0.53
34:BI:164:ASP:HB3	34:BI:211:GLN:HE21	1.72	0.53
52:BP:141:TYR:CG	52:BP:141:TYR:O	2.61	0.53
65:BL:169:LYS:HB3	65:BL:283:TYR:CE2	2.42	0.53
71:1:73:G:H3'	71:1:74:A:C8	2.43	0.53
71:1:155:U:H2'	71:1:156:A:O4'	2.08	0.53
71:1:392:A:O2'	71:1:997:A:N3	2.39	0.53
71:1:548:A:O2'	71:1:549:C:O4'	2.27	0.53
1:A:86:TYR:O	50:BE:112:THR:OG1	2.23	0.53
2:B:142:GLU:OE1	2:B:144:ARG:N	2.35	0.53
44:BM:126:LEU:O	44:BM:130:GLN:N	2.41	0.53
44:BM:377:GLU:O	44:BM:381:ASN:ND2	2.41	0.53
52:BP:168:SER:O	52:BP:170:ASN:N	2.42	0.53
71:1:1008:A:H8	71:1:1009:A:H1'	1.73	0.53
9:I:152:ARG:NH1	9:I:157:ASN:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:38:ILE:HG22	10:J:43:MET:HG3	1.88	0.53
10:J:62:PHE:CE2	10:J:112:LYS:HD2	2.42	0.53
14:N:170:ILE:HD13	14:N:179:LEU:HD22	1.90	0.53
17:Q:74:ASP:OD2	26:Z:16:PRO:HA	2.08	0.53
21:U:55:LYS:O	21:U:60:ARG:HG3	2.09	0.53
22:V:62:MET:HA	22:V:77:ARG:HD2	1.91	0.53
22:V:104:ARG:NH1	71:1:184:G:O4'	2.41	0.53
44:BM:46:ARG:HH12	44:BM:47:LYS:HD3	1.73	0.53
47:BH:33:ILE:HG22	47:BH:40:LEU:HD12	1.90	0.53
71:1:69:G:H5"	71:1:70:G:O4'	2.07	0.53
71:1:482:C:H2'	71:1:483:U:H4'	1.89	0.53
2:B:384:ARG:NH1	18:R:212:SER:H	2.07	0.53
4:D:87:TYR:OH	5:E:172:PRO:HD3	2.08	0.53
5:E:149:LEU:HB2	5:E:191:ILE:HG22	1.91	0.53
10:J:65:ASN:HB3	66:BO:172:ARG:CD	2.38	0.53
14:N:77:ASN:HD21	71:1:87:A:H1'	1.73	0.53
16:P:123:ARG:HH12	47:BH:225:ILE:HB	1.72	0.53
21:U:32:ARG:HB3	22:V:65:ARG:HH22	1.69	0.53
29:BB:17:HIS:HD2	29:BB:24:ARG:HH22	1.57	0.53
34:BI:198:LEU:HD13	34:BI:214:ILE:HG12	1.91	0.53
71:1:269:A:H2	71:1:271:U:H1'	1.73	0.53
71:1:781:A:HO2'	71:1:782:U:P	2.31	0.53
1:A:169:ARG:NH2	71:1:1117:U:O2	2.41	0.53
8:H:99:GLU:HG3	71:1:390:A:C2	2.43	0.53
22:V:89:ARG:HG2	71:1:374:U:H5"	1.90	0.53
29:BB:131:PHE:CZ	50:BE:73:PHE:HB2	2.44	0.53
34:BI:115:LEU:HD21	34:BI:144:LEU:HD12	1.89	0.53
44:BM:31:ARG:O	44:BM:35:GLN:HG2	2.09	0.53
44:BM:104:ASP:N	44:BM:104:ASP:OD1	2.37	0.53
47:BH:32:ASP:HB2	47:BH:191:ASP:HB3	1.91	0.53
54:BF:22:HIS:HA	71:1:595:A:H61	1.74	0.53
65:BL:310:ARG:O	65:BL:312:SER:N	2.41	0.53
71:1:568:A:H2'	71:1:569:U:O4'	2.09	0.53
7:G:174:ARG:HH11	71:1:191:A:H3'	1.73	0.53
13:M:12:LEU:HD11	13:M:13:ARG:HD3	1.91	0.53
13:M:198:ARG:HD3	13:M:241:MET:SD	2.49	0.53
15:O:175:ASP:HA	15:O:190:GLN:HG2	1.91	0.53
15:O:282:GLN:HB2	34:BI:206:HIS:CD2	2.44	0.53
65:BL:215:THR:HG22	65:BL:269:ASN:HB2	1.89	0.53
71:1:1029:U:H3	71:1:1057:A:H61	1.54	0.53
2:B:324:ASP:N	2:B:324:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:PRO:HA	17:Q:110:TYR:CD2	2.44	0.53
4:D:100:ASP:O	4:D:103:ALA:N	2.42	0.53
16:P:53:PHE:HD1	16:P:56:ASP:H	1.57	0.53
18:R:243:ILE:HG13	18:R:257:GLY:H	1.74	0.53
20:T:79:ARG:O	20:T:82:LYS:NZ	2.35	0.53
24:X:75:LEU:HD13	24:X:80:PHE:HE2	1.73	0.53
27:BA:48:THR:H	27:BA:51:ASP:HB2	1.73	0.53
28:UA:195:UNK:O	28:UA:199:UNK:N	2.42	0.53
34:BI:97:THR:HB	34:BI:234:VAL:HG12	1.90	0.53
65:BL:139:ARG:NH2	65:BL:299:PRO:HG3	2.24	0.53
66:BO:91:CYS:O	66:BO:95:PRO:HD3	2.09	0.53
71:1:132:U:H5"	71:1:133:A:C2	2.42	0.53
2:B:167:ARG:NH2	71:1:528:A:OP1	2.42	0.53
7:G:254:ASN:HD21	7:G:288:PHE:HB3	1.74	0.53
7:G:359:HIS:HB2	17:Q:12:THR:HG21	1.91	0.53
8:H:123:PHE:HE2	8:H:149:ILE:HD11	1.74	0.53
10:J:121:SER:HG	10:J:124:HIS:H	1.54	0.53
27:BA:42:SER:HB3	27:BA:131:ARG:HH22	1.73	0.53
44:BM:280:LEU:H	44:BM:280:LEU:HD23	1.73	0.53
54:BF:32:LEU:O	54:BF:36:ALA:N	2.31	0.53
71:1:643:G:O3'	71:1:656:G:N2	2.42	0.53
15:O:29:ARG:CD	15:O:29:ARG:N	2.66	0.53
15:O:269:ARG:HG2	15:O:273:MET:HG3	1.91	0.53
22:V:39:VAL:HG21	71:1:98:G:C8	2.44	0.53
37:BC:53:ALA:HB2	37:BC:90:GLN:O	2.09	0.53
44:BM:240:ASP:HB3	44:BM:279:TYR:CE2	2.44	0.53
47:BH:94:ASP:OD2	47:BH:141:GLN:NE2	2.41	0.53
65:BL:112:SER:OG	65:BL:112:SER:O	2.25	0.53
69:UC:88:UNK:O	69:UC:92:UNK:N	2.42	0.53
1:A:168:THR:OG1	1:A:169:ARG:N	2.42	0.52
7:G:282:ARG:HA	7:G:285:LEU:HD12	1.90	0.52
11:K:31:GLU:OE1	71:1:172:A:H4'	2.09	0.52
25:Y:167:LEU:HD13	25:Y:180:VAL:HG11	1.91	0.52
44:BM:97:GLY:O	44:BM:101:LYS:N	2.42	0.52
2:B:78:PRO:HB2	2:B:361:PHE:CE2	2.43	0.52
8:H:131:ARG:HD3	71:1:450:A:H5'	1.91	0.52
17:Q:81:ARG:HH21	71:1:81:U:H5	1.57	0.52
17:Q:108:ILE:HB	71:1:905:A:N6	2.16	0.52
22:V:82:PRO:HD3	24:X:458:VAL:HG11	1.91	0.52
24:X:170:VAL:HG23	24:X:223:SER:HB2	1.92	0.52
44:BM:67:GLU:H	44:BM:319:ALA:HB1	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:99:A:H4'	71:1:100:A:C5'	2.39	0.52
71:1:393:A:H4'	71:1:1012:A:N6	2.24	0.52
71:1:573:A:O2'	71:1:574:A:OP1	2.21	0.52
71:1:608:A:O2'	71:1:817:A:N6	2.43	0.52
14:N:194:ARG:HD3	71:1:565:U:N3	2.25	0.52
54:BF:63:ARG:NH1	54:BF:68:GLN:HA	2.24	0.52
67:BG:1298:PHE:O	67:BG:1298:PHE:CG	2.60	0.52
71:1:166:U:H5'	71:1:167:U:OP2	2.09	0.52
71:1:433:G:HO2'	71:1:434:U:P	2.32	0.52
71:1:504:U:O2'	71:1:505:A:OP2	2.24	0.52
71:1:508:G:H1'	71:1:509:U:OP2	2.09	0.52
71:1:654:A:H2'	71:1:655:U:H5"	1.92	0.52
3:C:116:ILE:HD11	3:C:162:TYR:CE1	2.44	0.52
4:D:100:ASP:OD1	4:D:101:ARG:N	2.42	0.52
13:M:215:ILE:HG23	71:1:577:A:C6	2.44	0.52
14:N:78:ARG:HH21	14:N:79:ASP:H	1.55	0.52
14:N:85:ARG:NE	71:1:313:A:O3'	2.41	0.52
24:X:49:ARG:O	24:X:53:GLN:HG2	2.10	0.52
71:1:433:G:O2'	71:1:434:U:H3'	2.09	0.52
71:1:929:G:H4'	71:1:930:A:C8	2.45	0.52
71:1:1131:A:N6	71:1:1147:A:H61	2.07	0.52
71:1:1136:U:H5	71:1:1142:U:N3	2.08	0.52
1:A:236:GLU:HA	1:A:305:PRO:HA	1.91	0.52
13:M:205:MET:HE3	71:1:134:A:H5"	1.92	0.52
15:O:89:HIS:CD2	15:O:91:LYS:H	2.27	0.52
15:O:91:LYS:NZ	71:1:541:U:O2	2.39	0.52
18:R:190:GLN:O	18:R:194:GLN:NE2	2.42	0.52
21:U:25:PHE:CB	71:1:972:A:N6	2.62	0.52
22:V:32:PHE:HD2	22:V:98:LYS:NZ	2.08	0.52
50:BE:110:SER:OG	50:BE:113:HIS:N	2.26	0.52
66:BO:97:VAL:O	66:BO:99:HIS:ND1	2.43	0.52
71:1:689:U:HO2'	71:1:690:U:P	2.33	0.52
71:1:981:A:O2'	71:1:1086:U:O2'	2.28	0.52
6:F:159:THR:HG22	6:F:159:THR:O	2.09	0.52
7:G:34:LEU:HD12	7:G:39:ASN:HD21	1.74	0.52
7:G:79:TRP:HD1	7:G:96:TYR:CE2	2.27	0.52
7:G:130:TYR:CE2	7:G:134:ARG:HD2	2.44	0.52
12:L:95:LEU:HD11	12:L:104:LEU:HD21	1.92	0.52
16:P:160:GLU:O	16:P:163:GLN:NE2	2.42	0.52
17:Q:142:LYS:HE2	17:Q:143:ARG:NH1	2.24	0.52
21:U:25:PHE:CE1	71:1:950:A:C6	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BC:95:LEU:HD13	37:BC:121:LEU:HD11	1.92	0.52
65:BL:205:LEU:HD22	65:BL:210:GLN:NE2	2.24	0.52
66:BO:94:PHE:HE2	71:1:1128:U:H3'	1.74	0.52
71:1:1068:A:H2'	71:1:1096:A:H61	1.74	0.52
3:C:75:PRO:HG2	3:C:76:HIS:CD2	2.44	0.52
14:N:112:VAL:CG2	18:R:397:PRO:HB2	2.39	0.52
24:X:274:LEU:HD11	24:X:278:ARG:HD3	1.92	0.52
26:Z:152:ARG:HD2	26:Z:154:LYS:HE3	1.90	0.52
28:UA:59:UNK:O	28:UA:63:UNK:N	2.43	0.52
34:BI:158:TYR:HA	34:BI:217:ALA:HB2	1.92	0.52
71:1:507:U:O2'	71:1:510:U:H4'	2.09	0.52
71:1:554:G:O2'	71:1:555:U:O5'	2.28	0.52
71:1:681:G:N2	71:1:793:C:N3	2.51	0.52
71:1:711:A:O2'	71:1:749:U:O4'	2.26	0.52
71:1:1157:A:O2'	71:1:1158:U:OP1	2.26	0.52
1:A:387:PHE:CE2	66:BO:93:VAL:HG11	2.44	0.52
2:B:210:GLN:HA	7:G:89:GLN:HE22	1.74	0.52
3:C:52:TRP:O	3:C:56:ALA:N	2.43	0.52
8:H:11:LEU:HB3	8:H:17:TYR:CE1	2.45	0.52
9:I:59:ARG:NH1	71:1:821:U:OP2	2.42	0.52
14:N:47:ARG:HG3	71:1:90:A:OP1	2.09	0.52
16:P:53:PHE:HB3	16:P:60:ARG:NE	2.25	0.52
18:R:406:TYR:O	18:R:410:THR:HG22	2.10	0.52
24:X:49:ARG:O	24:X:53:GLN:N	2.43	0.52
24:X:491:GLN:NE2	24:X:500:THR:OG1	2.42	0.52
37:BC:117:THR:HG23	37:BC:120:LEU:H	1.74	0.52
50:BE:36:THR:O	50:BE:38:ASP:N	2.42	0.52
65:BL:84:GLN:HG3	65:BL:291:LYS:HG3	1.91	0.52
71:1:401:U:O2'	71:1:402:U:OP2	2.25	0.52
71:1:593:U:HO2'	71:1:594:U:P	2.32	0.52
2:B:181:VAL:HG23	2:B:186:LEU:HD21	1.92	0.52
10:J:104:ILE:HG22	10:J:106:ALA:H	1.75	0.52
13:M:251:TYR:OH	70:UD:72:UNK:HA	2.10	0.52
18:R:404:TYR:CD2	71:1:60:A:C4	2.98	0.52
26:Z:25:PHE:O	26:Z:28:THR:N	2.40	0.52
27:BA:22:PRO:O	27:BA:26:LYS:HB2	2.09	0.52
71:1:58:A:HO2'	71:1:112:U:HO2'	1.53	0.52
71:1:225:U:H2'	71:1:226:A:C8	2.41	0.52
71:1:639:A:H61	71:1:799:A:N6	2.07	0.52
71:1:697:A:H4'	71:1:698:G:OP2	2.10	0.52
71:1:871:A:N7	71:1:1064:G:O2'	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:1131:A:H61	71:1:1147:A:H61	1.56	0.52
1:A:207:HIS:HD2	1:A:329:TYR:OH	1.93	0.52
3:C:125:GLU:OE1	3:C:126:ARG:HG3	2.10	0.52
7:G:153:LEU:O	7:G:153:LEU:HD13	2.10	0.52
7:G:209:ARG:HD3	71:1:190:A:H2	1.75	0.52
12:L:97:SER:HB3	12:L:104:LEU:HD12	1.91	0.52
21:U:18:LEU:CD2	21:U:19:LYS:H	2.23	0.52
22:V:10:PRO:N	22:V:14:CYS:HA	2.25	0.52
34:BI:86:ILE:HG21	34:BI:243:ILE:HD11	1.92	0.52
44:BM:71:ARG:O	44:BM:75:VAL:HG23	2.10	0.52
66:BO:107:LYS:HG3	66:BO:108:GLY:N	2.25	0.52
66:BO:176:HIS:CD2	66:BO:178:TYR:H	2.27	0.52
71:1:235:G:C2	71:1:236:A:C5	2.98	0.52
71:1:248:U:N3	71:1:250:A:N1	2.58	0.52
71:1:681:G:H1	71:1:793:C:N4	2.08	0.52
71:1:828:A:H2	71:1:1099:A:H62	1.58	0.52
1:A:60:HIS:CD2	1:A:65:SER:HB3	2.45	0.51
2:B:127:TYR:CD1	2:B:189:PRO:HG2	2.45	0.51
3:C:102:ILE:HG13	17:Q:83:ARG:HE	1.75	0.51
5:E:221:HIS:O	5:E:225:TYR:N	2.35	0.51
18:R:297:GLN:HB3	18:R:303:ASN:O	2.10	0.51
26:Z:152:ARG:HH11	26:Z:154:LYS:HE3	1.75	0.51
34:BI:117:THR:HG22	34:BI:265:LYS:HB2	1.92	0.51
61:BD:31:ASN:ND2	61:BD:34:LEU:HG	2.24	0.51
65:BL:236:ILE:HG13	65:BL:267:PHE:HZ	1.75	0.51
66:BO:68:CYS:H	66:BO:76:HIS:HB2	1.75	0.51
1:A:152:ASP:OD2	9:I:11:ARG:NH1	2.43	0.51
5:E:177:VAL:HA	5:E:180:VAL:HG12	1.92	0.51
8:H:117:THR:OG1	8:H:118:THR:N	2.44	0.51
9:I:42:GLU:HB3	9:I:45:MET:CG	2.40	0.51
16:P:55:GLN:HG2	71:1:949:U:O2	2.10	0.51
34:BI:152:HIS:CE1	34:BI:162:GLY:HA2	2.46	0.51
71:1:1074:A:H1'	71:1:1075:A:P	2.50	0.51
16:P:112:ARG:NH1	47:BH:219:LYS:HG2	2.26	0.51
18:R:412:LYS:HD3	18:R:451:CYS:HB3	1.92	0.51
22:V:119:GLN:NE2	22:V:123:LEU:HD21	2.25	0.51
24:X:481:LEU:HD12	24:X:482:PRO:HD2	1.93	0.51
44:BM:148:ALA:HB1	44:BM:255:ARG:HH11	1.75	0.51
71:1:760:A:OP2	71:1:1079:A:O2'	2.17	0.51
1:A:84:THR:OG1	50:BE:89:GLU:OE2	2.26	0.51
2:B:14:PRO:HG2	13:M:105:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:58:LYS:HG3	6:F:59:ASP:OD1	2.10	0.51
9:I:57:LYS:NZ	71:1:819:U:OP2	2.44	0.51
15:O:217:LYS:HD3	15:O:228:GLU:HA	1.93	0.51
21:U:45:ALA:O	21:U:47:THR:N	2.35	0.51
71:1:766:A:H2'	71:1:767:U:O4'	2.11	0.51
71:1:1113:G:C6	71:1:1114:A:C2	2.98	0.51
2:B:402:HIS:N	2:B:403:PRO:CD	2.74	0.51
4:D:76:GLU:CD	4:D:76:GLU:H	2.12	0.51
5:E:275:LYS:HD2	5:E:327:MET:HB2	1.93	0.51
6:F:114:LYS:O	6:F:118:ARG:HG3	2.09	0.51
11:K:67:ASP:O	11:K:71:HIS:N	2.42	0.51
11:K:176:THR:O	11:K:179:TRP:N	2.43	0.51
24:X:142:ALA:O	24:X:146:GLN:N	2.36	0.51
44:BM:46:ARG:HH21	44:BM:50:LYS:NZ	2.08	0.51
66:BO:80:ILE:HD13	66:BO:100:ARG:NH1	2.25	0.51
1:A:392:LEU:HD13	10:J:64:TYR:HD2	1.74	0.51
2:B:33:HIS:ND1	2:B:34:PRO:HD2	2.26	0.51
18:R:195:TYR:OH	18:R:199:ARG:HD2	2.11	0.51
20:T:72:TRP:CD1	20:T:83:PRO:HD2	2.46	0.51
37:BC:29:THR:OG1	37:BC:34:GLU:O	2.28	0.51
71:1:969:U:H2'	71:1:970:A:C8	2.45	0.51
1:A:393:VAL:HG12	66:BO:180:LEU:HD23	1.92	0.51
5:E:136:THR:HA	5:E:146:CYS:SG	2.51	0.51
9:I:156:ASP:OD1	9:I:156:ASP:N	2.40	0.51
10:J:103:TRP:HE1	66:BO:144:GLN:NE2	2.09	0.51
13:M:145:LYS:O	13:M:148:ILE:HG12	2.11	0.51
22:V:43:ARG:NH1	71:1:97:U:O2	2.44	0.51
24:X:249:LYS:HB2	24:X:253:HIS:HA	1.92	0.51
65:BL:114:ASP:CG	65:BL:114:ASP:O	2.48	0.51
71:1:572:A:H4'	71:1:573:A:OP2	2.10	0.51
71:1:575:G:H5'	71:1:576:A:OP2	2.11	0.51
71:1:1037:C:N4	71:1:1127:U:OP2	2.43	0.51
71:1:1077:G:H1	71:1:1090:U:H3	1.58	0.51
8:H:45:ILE:HD11	8:H:157:PRO:O	2.11	0.51
15:O:107:ALA:O	15:O:108:ARG:HG3	2.11	0.51
17:Q:115:ASP:OD2	17:Q:163:ARG:NH2	2.43	0.51
18:R:190:GLN:HG2	18:R:194:GLN:HE22	1.75	0.51
21:U:92:PHE:HE2	71:1:965:G:H21	1.58	0.51
22:V:53:ARG:HH21	22:V:109:ARG:NH1	2.08	0.51
25:Y:148:PRO:HA	25:Y:151:ARG:HH11	1.75	0.51
28:UA:189:UNK:O	28:UA:193:UNK:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BB:54:VAL:HG23	29:BB:56:PRO:CD	2.39	0.51
37:BC:4:ILE:HG23	37:BC:7:ARG:HH21	1.75	0.51
50:BE:67:LYS:HD2	50:BE:67:LYS:O	2.10	0.51
65:BL:107:TRP:CD1	65:BL:138:VAL:HG21	2.45	0.51
65:BL:158:TRP:CD1	65:BL:176:LEU:HD12	2.45	0.51
65:BL:189:TYR:HB3	65:BL:277:ARG:HB2	1.92	0.51
71:1:1143:A:C6	71:1:1144:G:C2	2.99	0.51
2:B:295:SER:OG	2:B:295:SER:O	2.18	0.51
3:C:120:ASN:HD22	3:C:129:TRP:HZ3	1.59	0.51
5:E:59:ALA:O	5:E:90:THR:OG1	2.23	0.51
26:Z:44:LEU:HG	26:Z:44:LEU:O	2.10	0.51
29:BB:13:LYS:NZ	71:1:1120:U:OP1	2.33	0.51
29:BB:129:THR:HB	50:BE:73:PHE:HB3	1.93	0.51
34:BI:201:ALA:HB3	34:BI:211:GLN:HB3	1.93	0.51
6:F:168:GLN:NE2	71:1:490:U:OP2	2.44	0.51
9:I:244:SER:HB2	54:BF:70:ARG:HH22	1.75	0.51
12:L:35:SER:HB3	12:L:38:ASP:HB2	1.92	0.51
13:M:259:ARG:NE	70:UD:15:UNK:O	2.43	0.51
14:N:50:ARG:HB2	22:V:28:PRO:O	2.11	0.51
14:N:196:ARG:CZ	71:1:563:U:H5'	2.41	0.51
15:O:129:TYR:O	15:O:164:ASN:ND2	2.32	0.51
15:O:282:GLN:HB2	34:BI:206:HIS:NE2	2.26	0.51
22:V:116:ASP:O	22:V:119:GLN:HB3	2.10	0.51
25:Y:51:LYS:HZ3	25:Y:53:HIS:HB3	1.74	0.51
34:BI:174:LEU:O	34:BI:210:SER:N	2.44	0.51
44:BM:32:PHE:O	44:BM:36:VAL:HG23	2.11	0.51
65:BL:152:GLN:NE2	65:BL:177:TYR:OH	2.45	0.51
71:1:847:A:C8	71:1:848:U:H5	2.28	0.51
71:1:1105:G:C2	71:1:1106:U:C4	2.98	0.51
1:A:62:ASP:OD1	1:A:63:LYS:N	2.44	0.50
9:I:103:LEU:HD21	9:I:114:GLN:OE1	2.11	0.50
12:L:29:ASN:ND2	12:L:29:ASN:O	2.44	0.50
13:M:254:LEU:HD13	70:UD:12:UNK:HA	1.93	0.50
24:X:353:PRO:HD3	24:X:393:CYS:HA	1.93	0.50
24:X:355:THR:OG1	24:X:356:ALA:N	2.44	0.50
25:Y:118:LEU:HD21	37:BC:74:LEU:HD12	1.92	0.50
34:BI:85:ASP:HB3	34:BI:93:PRO:HB3	1.93	0.50
44:BM:227:TYR:HA	44:BM:230:VAL:HG22	1.93	0.50
47:BH:69:TYR:OH	71:1:360:U:O2	2.24	0.50
52:BP:-5:LYS:HD3	52:BP:0:TRP:CD1	2.46	0.50
65:BL:263:GLU:OE2	71:1:665:U:H2'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:618:U:OP1	71:1:1040:C:H5'	2.10	0.50
1:A:371:GLU:N	1:A:371:GLU:OE2	2.44	0.50
13:M:135:MET:HE3	13:M:137:LYS:HG2	1.94	0.50
24:X:89:LEU:HD21	24:X:125:HIS:NE2	2.26	0.50
24:X:293:ASN:H	24:X:344:GLN:NE2	2.09	0.50
25:Y:61:GLN:HA	25:Y:64:VAL:HG12	1.93	0.50
26:Z:44:LEU:O	26:Z:44:LEU:CG	2.59	0.50
44:BM:28:VAL:HB	44:BM:30:GLU:HG2	1.94	0.50
47:BH:150:GLU:OE1	47:BH:150:GLU:N	2.42	0.50
66:BO:138:THR:HG22	66:BO:144:GLN:HB3	1.92	0.50
71:1:408:U:H2'	71:1:409:A:C8	2.46	0.50
71:1:1031:C:N3	71:1:1035:G:N2	2.59	0.50
2:B:283:LEU:HB2	2:B:340:MET:HE3	1.93	0.50
5:E:37:ASP:OD1	5:E:38:ILE:N	2.44	0.50
5:E:50:LEU:HD11	5:E:108:PHE:HA	1.94	0.50
21:U:25:PHE:CE2	21:U:27:PRO:HB3	2.47	0.50
66:BO:79:LEU:HD12	66:BO:101:VAL:HG23	1.94	0.50
71:1:116:U:H2'	71:1:117:U:H5"	1.93	0.50
71:1:928:U:HO2'	71:1:929:G:P	2.28	0.50
1:A:330:VAL:HG13	1:A:332:PHE:HE1	1.76	0.50
2:B:387:GLU:HG3	18:R:222:TYR:HE2	1.76	0.50
9:I:214:SER:HB3	54:BF:29:ARG:HD3	1.92	0.50
10:J:108:ASN:HD22	10:J:111:LEU:HD22	1.76	0.50
17:Q:114:LEU:HD23	17:Q:114:LEU:H	1.77	0.50
24:X:260:THR:OG1	24:X:344:GLN:NE2	2.44	0.50
26:Z:44:LEU:O	26:Z:44:LEU:HD23	2.11	0.50
44:BM:325:GLN:HA	44:BM:328:TYR:CD2	2.47	0.50
65:BL:301:ARG:HH12	71:1:235:G:H5'	1.77	0.50
71:1:865:A:H4'	71:1:866:A:OP1	2.12	0.50
71:1:1080:A:H2'	71:1:1081:U:C6	2.46	0.50
1:A:353:PHE:HB3	1:A:354:PRO:HD3	1.94	0.50
1:A:390:ALA:HB1	71:1:1132:U:O2'	2.12	0.50
4:D:76:GLU:HA	4:D:79:PHE:HB3	1.92	0.50
5:E:186:ARG:HD2	71:1:452:A:C5	2.46	0.50
14:N:152:ARG:HG3	14:N:169:HIS:HB2	1.93	0.50
16:P:167:TYR:HB3	16:P:173:VAL:HG23	1.93	0.50
18:R:17:VAL:HG23	18:R:64:ILE:HD11	1.94	0.50
50:BE:60:LYS:HZ1	50:BE:67:LYS:HB3	1.75	0.50
50:BE:62:VAL:O	50:BE:64:ALA:N	2.45	0.50
71:1:991:G:N2	71:1:992:G:O4'	2.44	0.50
1:A:377:PRO:HD3	29:BB:106:PRO:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:SER:HB3	2:B:257:THR:CG2	2.42	0.50
3:C:90:TYR:HB3	3:C:91:PRO:HD2	1.93	0.50
8:H:19:HIS:HB3	8:H:22:THR:O	2.12	0.50
9:I:42:GLU:HB3	9:I:45:MET:SD	2.52	0.50
15:O:163:LYS:NZ	18:R:430:ASP:OD2	2.45	0.50
24:X:300:VAL:HB	24:X:306:ALA:HA	1.93	0.50
24:X:365:LEU:N	24:X:367:GLN:OE1	2.37	0.50
25:Y:241:PRO:HA	25:Y:244:ARG:HH12	1.76	0.50
66:BO:101:VAL:O	66:BO:103:VAL:N	2.44	0.50
71:1:757:A:O2'	71:1:758:G:H5'	2.11	0.50
71:1:1061:A:H3'	71:1:1062:U:H5"	1.93	0.50
1:A:312:LYS:HD2	1:A:367:LEU:HD12	1.94	0.50
6:F:29:ILE:HG13	6:F:145:TRP:CE2	2.46	0.50
7:G:221:GLY:HA2	71:1:202:A:OP1	2.12	0.50
12:L:2:LEU:HB2	12:L:125:PRO:HG2	1.94	0.50
12:L:45:LEU:O	12:L:47:ALA:N	2.45	0.50
13:M:20:ASN:OD1	71:1:326:U:O2'	2.30	0.50
13:M:143:TRP:CD1	13:M:206:PRO:HA	2.47	0.50
24:X:199:THR:HG23	24:X:202:ASN:H	1.76	0.50
24:X:340:LEU:HG	24:X:411:VAL:HG22	1.94	0.50
44:BM:15:ASN:HA	44:BM:20:LEU:HD22	1.93	0.50
44:BM:68:LEU:O	44:BM:69:LEU:HD23	2.12	0.50
50:BE:46:SER:HB2	50:BE:48:ALA:O	2.11	0.50
71:1:651:U:O2'	71:1:652:A:H5'	2.12	0.50
2:B:147:TRP:NE1	14:N:83:ASP:O	2.35	0.50
9:I:100:VAL:O	9:I:104:ALA:N	2.41	0.50
10:J:11:HIS:CD2	71:1:1113:G:H4'	2.47	0.50
13:M:14:PRO:O	13:M:14:PRO:CD	2.59	0.50
18:R:32:GLY:O	26:Z:156:TYR:HB2	2.12	0.50
25:Y:65:ASP:O	25:Y:69:SER:N	2.43	0.50
27:BA:68:VAL:HG12	27:BA:114:PHE:HB2	1.94	0.50
29:BB:19:VAL:HG12	29:BB:20:HIS:CD2	2.38	0.50
44:BM:224:PRO:HB2	44:BM:226:ASP:H	1.77	0.50
47:BH:202:GLU:HA	47:BH:205:GLU:OE2	2.12	0.50
54:BF:48:SER:HB2	54:BF:56:THR:HG21	1.93	0.50
65:BL:111:SER:OG	65:BL:112:SER:N	2.44	0.50
65:BL:340:VAL:O	65:BL:341:LYS:C	2.51	0.50
71:1:572:A:H3'	71:1:573:A:C8	2.46	0.50
71:1:646:U:H2'	71:1:647:U:H6	1.77	0.50
1:A:285:TYR:CD1	6:F:79:PRO:HG3	2.47	0.50
3:C:100:LEU:HD21	3:C:106:HIS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:139:VAL:O	5:E:143:GLY:N	2.40	0.50
5:E:153:MET:O	5:E:157:ILE:HD12	2.11	0.50
7:G:232:ILE:HD13	7:G:245:LEU:HD13	1.94	0.50
8:H:22:THR:HG21	8:H:24:ARG:HH21	1.76	0.50
9:I:185:ARG:CD	9:I:188:LEU:HD11	2.41	0.50
9:I:258:TRP:O	9:I:262:MET:HG3	2.11	0.50
11:K:168:LEU:HD12	11:K:179:TRP:HE3	1.76	0.50
12:L:92:VAL:HG21	71:1:407:C:OP1	2.11	0.50
13:M:17:LYS:NZ	71:1:177:G:OP1	2.44	0.50
13:M:203:THR:HG21	15:O:31:ARG:NE	2.27	0.50
13:M:210:ASP:OD1	13:M:211:LYS:N	2.45	0.50
17:Q:62:PRO:HD2	71:1:81:U:C2	2.47	0.50
18:R:208:TRP:HD1	18:R:213:THR:CG2	2.25	0.50
28:UA:8:UNK:HA	67:BG:1274:ASN:HD21	1.77	0.50
54:BF:22:HIS:CD2	71:1:595:A:H62	2.30	0.50
66:BO:85:ALA:O	66:BO:86:GLU:HG3	2.11	0.50
66:BO:92:ARG:HA	66:BO:92:ARG:NE	2.26	0.50
66:BO:183:VAL:O	66:BO:183:VAL:HG12	2.12	0.50
71:1:562:U:H4'	71:1:563:U:OP2	2.10	0.50
71:1:632:A:H2'	71:1:632:A:OP2	2.12	0.50
9:I:185:ARG:HD2	9:I:188:LEU:CD1	2.41	0.49
10:J:65:ASN:HD22	66:BO:189:PHE:HD2	1.57	0.49
13:M:143:TRP:HB3	15:O:36:PHE:CZ	2.47	0.49
24:X:320:VAL:HG12	24:X:321:VAL:HG23	1.94	0.49
29:BB:21:LEU:O	29:BB:25:LEU:HG	2.12	0.49
29:BB:88:ARG:NH2	29:BB:89:GLU:HG2	2.26	0.49
54:BF:96:ARG:HA	54:BF:100:VAL:HG12	1.93	0.49
65:BL:119:ARG:NH1	65:BL:132:HIS:C	2.58	0.49
71:1:830:A:H3'	71:1:831:A:C8	2.47	0.49
71:1:1032:A:H2'	71:1:1033:U:H5"	1.93	0.49
8:H:27:ARG:NH2	8:H:96:LYS:HG2	2.16	0.49
9:I:186:PHE:HE1	9:I:216:PHE:CE2	2.30	0.49
24:X:363:PHE:CE1	24:X:387:PRO:HD3	2.47	0.49
25:Y:169:PHE:CD1	37:BC:139:PRO:HD2	2.47	0.49
44:BM:329:THR:O	44:BM:333:ILE:HG13	2.12	0.49
61:BD:80:GLN:NE2	61:BD:80:GLN:O	2.45	0.49
65:BL:121:GLY:HA2	65:BL:130:LEU:O	2.12	0.49
71:1:341:U:H4'	71:1:973:U:C5	2.47	0.49
71:1:665:U:O4'	71:1:670:A:N6	2.45	0.49
71:1:827:A:HO2'	71:1:828:A:P	2.35	0.49
1:A:176:ASP:HB3	1:A:219:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:106:HIS:ND1	3:C:106:HIS:O	2.45	0.49
7:G:146:LYS:HE3	71:1:345:A:O2'	2.12	0.49
8:H:56:PHE:HE1	52:BP:183:ILE:HD13	1.77	0.49
9:I:80:LYS:HA	9:I:174:HIS:HE1	1.77	0.49
9:I:214:SER:HA	9:I:217:LYS:HE2	1.94	0.49
11:K:88:ASN:OD1	52:BP:6:HIS:HE1	1.95	0.49
15:O:197:VAL:HA	15:O:200:VAL:HG22	1.94	0.49
15:O:299:HIS:NE2	18:R:381:GLU:OE1	2.46	0.49
19:S:248:ALA:HB2	27:BA:66:ALA:H	1.77	0.49
25:Y:200:HIS:CD2	25:Y:221:VAL:HG11	2.47	0.49
26:Z:67:ASN:HB3	26:Z:121:LEU:HB2	1.94	0.49
28:UA:88:UNK:O	28:UA:92:UNK:N	2.45	0.49
44:BM:271:ARG:O	44:BM:275:SER:N	2.43	0.49
65:BL:128:VAL:O	65:BL:128:VAL:CG2	2.60	0.49
66:BO:132:THR:HG21	66:BO:147:PHE:CE2	2.47	0.49
71:1:127:A:H2'	71:1:128:U:H5'	1.94	0.49
71:1:302:A:C6	71:1:303:U:C4	3.00	0.49
71:1:509:U:C4	71:1:513:U:O2	2.66	0.49
71:1:1141:A:C6	71:1:1142:U:C2	3.01	0.49
2:B:82:THR:HG21	2:B:347:MET:HE3	1.94	0.49
3:C:172:HIS:ND1	3:C:196:GLU:OE2	2.43	0.49
6:F:113:ARG:NH1	71:1:150:A:O2'	2.44	0.49
8:H:96:LYS:HB3	8:H:99:GLU:HB2	1.93	0.49
11:K:53:GLN:HE22	71:1:489:A:H61	1.60	0.49
12:L:159:ASP:OD1	12:L:159:ASP:N	2.44	0.49
13:M:71:TRP:CZ2	13:M:77:LEU:HD22	2.47	0.49
13:M:170:ARG:HD2	13:M:173:HIS:CD2	2.48	0.49
24:X:187:ASP:OD1	24:X:188:LYS:N	2.45	0.49
24:X:250:GLN:HA	24:X:253:HIS:HB3	1.94	0.49
25:Y:237:LEU:HD23	37:BC:31:VAL:HG22	1.94	0.49
29:BB:20:HIS:HA	29:BB:23:ARG:HB2	1.94	0.49
44:BM:80:ARG:NH2	44:BM:83:TYR:HB2	2.27	0.49
71:1:398:U:HO2'	71:1:399:U:P	2.33	0.49
71:1:753:U:C4	71:1:754:A:C6	3.01	0.49
71:1:1121:U:H4'	71:1:1122:A:OP1	2.11	0.49
5:E:302:THR:N	5:E:305:GLU:OE2	2.45	0.49
8:H:32:TYR:O	8:H:115:LYS:NZ	2.38	0.49
13:M:12:LEU:CD1	13:M:13:ARG:HD3	2.43	0.49
13:M:213:VAL:HG22	13:M:223:TRP:CZ3	2.46	0.49
18:R:207:LYS:HZ2	18:R:314:ALA:H	1.59	0.49
25:Y:195:GLN:O	25:Y:199:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BL:119:ARG:NH1	65:BL:132:HIS:O	2.40	0.49
66:BO:87:ARG:HE	66:BO:89:ALA:HB3	1.77	0.49
71:1:410:A:HO2'	71:1:411:U:P	2.35	0.49
71:1:425:A:H8	71:1:471:A:H5"	1.77	0.49
71:1:649:A:N6	71:1:1073:A:H2'	2.28	0.49
71:1:750:U:H4'	71:1:751:A:C8	2.48	0.49
2:B:184:TRP:HB2	22:V:26:LEU:HD13	1.93	0.49
2:B:189:PRO:HG3	13:M:5:ALA:HB2	1.95	0.49
2:B:384:ARG:HH11	18:R:212:SER:H	1.59	0.49
5:E:54:ARG:NE	71:1:434:U:H5'	2.28	0.49
5:E:280:GLN:HE22	5:E:333:GLN:HA	1.78	0.49
7:G:188:ARG:NH2	71:1:188:A:OP2	2.38	0.49
12:L:62:GLY:HA2	12:L:67:THR:HA	1.94	0.49
24:X:439:ASP:HB3	24:X:442:ILE:HB	1.95	0.49
66:BO:109:ARG:HA	66:BO:109:ARG:NE	2.28	0.49
69:UC:131:UNK:O	69:UC:135:UNK:N	2.44	0.49
71:1:164:U:O2'	71:1:165:G:OP1	2.30	0.49
71:1:226:A:H61	71:1:310:A:N6	2.10	0.49
71:1:463:U:C2	71:1:465:A:H5"	2.47	0.49
1:A:329:TYR:CZ	10:J:17:ALA:HB2	2.47	0.49
5:E:105:GLN:HE22	71:1:429:A:H1'	1.75	0.49
9:I:29:ASP:OD1	9:I:29:ASP:N	2.43	0.49
9:I:180:THR:HG22	20:T:75:ARG:HA	1.93	0.49
9:I:238:ARG:HG2	15:O:94:ASP:OD2	2.12	0.49
15:O:267:TYR:CE2	15:O:269:ARG:HB2	2.48	0.49
18:R:12:ALA:O	18:R:15:GLU:HG2	2.12	0.49
27:BA:112:GLU:HG2	27:BA:112:GLU:O	2.13	0.49
28:UA:159:UNK:O	28:UA:163:UNK:N	2.46	0.49
52:BP:179:PRO:HG2	52:BP:181:ASN:HB3	1.93	0.49
65:BL:75:ASP:OD2	65:BL:280:GLY:HA2	2.13	0.49
66:BO:68:CYS:N	66:BO:76:HIS:HB2	2.28	0.49
71:1:219:A:O4'	71:1:319:A:N6	2.40	0.49
71:1:1125:U:O2'	71:1:1126:A:OP1	2.31	0.49
2:B:94:VAL:HG22	2:B:103:HIS:O	2.13	0.49
2:B:254:SER:HB3	2:B:257:THR:HG22	1.94	0.49
7:G:262:LEU:O	7:G:266:LEU:HG	2.12	0.49
7:G:336:TYR:O	7:G:340:LYS:N	2.40	0.49
9:I:72:ARG:NH2	71:1:543:U:O2'	2.46	0.49
15:O:289:VAL:HA	15:O:292:LEU:HB2	1.95	0.49
21:U:50:MET:O	71:1:965:G:O2'	2.27	0.49
24:X:349:PRO:CD	24:X:398:ARG:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:205:GLU:HG3	25:Y:206:ALA:N	2.28	0.49
27:BA:115:VAL:HG23	27:BA:140:ALA:O	2.12	0.49
29:BB:18:ARG:NH1	71:1:1118:G:N7	2.60	0.49
44:BM:68:LEU:HD13	44:BM:72:TYR:HD2	1.78	0.49
44:BM:330:SER:HB2	44:BM:331:PRO:HD3	1.95	0.49
47:BH:82:HIS:CE1	47:BH:91:GLN:HG2	2.48	0.49
47:BH:188:TRP:CE3	47:BH:227:PRO:HB3	2.47	0.49
65:BL:214:LEU:HB3	65:BL:255:VAL:HG11	1.94	0.49
71:1:425:A:H2'	71:1:425:A:N3	2.27	0.49
71:1:456:A:H1'	71:1:457:C:H5'	1.94	0.49
71:1:871:A:H2'	71:1:872:A:C4	2.48	0.49
4:D:134:LEU:HB2	4:D:135:PRO:HD3	1.95	0.49
8:H:27:ARG:HH12	8:H:96:LYS:HA	1.77	0.49
12:L:135:ASP:O	12:L:137:VAL:HG22	2.13	0.49
18:R:20:ASN:OD1	18:R:21:PHE:N	2.45	0.49
24:X:173:GLY:HA3	24:X:205:PHE:CD2	2.47	0.49
24:X:290:MET:SD	24:X:400:VAL:HG21	2.52	0.49
25:Y:162:ARG:HB2	25:Y:163:PRO:HD2	1.95	0.49
25:Y:234:ILE:O	25:Y:238:HIS:N	2.45	0.49
44:BM:51:GLU:OE2	44:BM:312:VAL:HG23	2.13	0.49
44:BM:89:ARG:O	44:BM:92:THR:OG1	2.29	0.49
65:BL:90:PRO:O	65:BL:91:PHE:HB2	2.13	0.49
66:BO:129:CYS:HB3	66:BO:153:ILE:HG13	1.95	0.49
71:1:320:G:N2	71:1:322:A:O3'	2.45	0.49
71:1:482:C:H2'	71:1:483:U:C4'	2.42	0.49
71:1:559:U:O2'	71:1:560:U:H3'	2.13	0.49
71:1:643:G:H2'	71:1:644:C:O4'	2.13	0.49
2:B:50:SER:OG	2:B:211:GLY:O	2.29	0.49
2:B:147:TRP:HH2	14:N:87:PHE:CD2	2.31	0.49
7:G:227:PRO:HG2	7:G:228:TYR:CE2	2.48	0.49
7:G:366:MET:SD	17:Q:28:ARG:NH1	2.69	0.49
8:H:81:ALA:O	8:H:126:THR:HG22	2.13	0.49
15:O:137:TYR:HB3	15:O:138:PRO:HD2	1.95	0.49
27:BA:49:SER:OG	27:BA:50:ALA:N	2.46	0.49
34:BI:147:ARG:HH11	34:BI:148:ASN:ND2	2.11	0.49
47:BH:101:ARG:NH2	71:1:365:U:O2	2.46	0.49
52:BP:8:ASP:OD2	71:1:491:U:O2'	2.26	0.49
65:BL:116:PHE:O	65:BL:118:HIS:CD2	2.66	0.49
65:BL:241:GLY:HA3	71:1:671:U:C4	2.48	0.49
71:1:47:A:N6	71:1:131:U:H3	2.11	0.49
71:1:299:U:H4'	71:1:300:A:O5'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLN:HB3	1:A:206:LYS:HE3	1.94	0.48
1:A:299:GLU:HG2	1:A:300:THR:H	1.78	0.48
5:E:58:LYS:NZ	5:E:97:ASP:OD2	2.45	0.48
8:H:93:VAL:HG12	8:H:94:VAL:H	1.78	0.48
13:M:118:LEU:O	13:M:121:GLU:N	2.45	0.48
15:O:204:ASP:HB3	15:O:207:THR:HB	1.95	0.48
18:R:247:CYS:HA	18:R:252:ASN:HA	1.94	0.48
21:U:54:ILE:O	21:U:54:ILE:HG13	2.12	0.48
21:U:72:MET:HB2	21:U:83:MET:HG3	1.95	0.48
22:V:116:ASP:HA	22:V:119:GLN:HB3	1.94	0.48
44:BM:158:MET:HG3	44:BM:217:LYS:NZ	2.27	0.48
71:1:269:A:C2	71:1:271:U:H1'	2.47	0.48
71:1:390:A:H2	71:1:391:A:C8	2.30	0.48
71:1:1013:U:H5"	71:1:1014:U:C4	2.48	0.48
1:A:166:HIS:ND1	1:A:178:VAL:HG22	2.28	0.48
3:C:70:ARG:NH1	3:C:70:ARG:HB2	2.28	0.48
26:Z:154:LYS:HB3	26:Z:155:PRO:HD2	1.96	0.48
44:BM:45:SER:CB	44:BM:118:ILE:HD13	2.43	0.48
61:BD:13:CYS:SG	61:BD:14:GLY:N	2.86	0.48
66:BO:172:ARG:NH2	66:BO:172:ARG:CB	2.76	0.48
71:1:55:A:H2'	71:1:56:U:O4'	2.14	0.48
71:1:120:A:H2	71:1:121:U:C5	2.30	0.48
71:1:433:G:HO2'	71:1:434:U:H3'	1.78	0.48
71:1:450:A:O2'	71:1:451:A:H4'	2.13	0.48
71:1:643:G:OP2	71:1:680:A:C4	2.66	0.48
71:1:935:G:N2	71:1:936:G:C4	2.81	0.48
71:1:1023:A:H2'	71:1:1024:U:O4'	2.13	0.48
2:B:287:GLU:OE1	2:B:288:PRO:HD2	2.13	0.48
7:G:174:ARG:HA	7:G:217:VAL:HG13	1.94	0.48
9:I:150:LYS:HA	20:T:71:GLU:HB3	1.95	0.48
9:I:256:GLU:HA	9:I:259:HIS:CD2	2.48	0.48
15:O:29:ARG:HB2	15:O:32:THR:HG1	1.77	0.48
18:R:167:HIS:HD2	18:R:169:GLY:N	2.05	0.48
20:T:35:PRO:O	20:T:39:ARG:N	2.44	0.48
22:V:48:GLY:HA2	24:X:459:ARG:O	2.14	0.48
24:X:300:VAL:HB	24:X:305:GLY:O	2.14	0.48
29:BB:120:VAL:HG13	29:BB:122:ASP:H	1.78	0.48
47:BH:84:ILE:HG23	47:BH:90:MET:HG2	1.94	0.48
65:BL:281:VAL:O	65:BL:282:MET:HB2	2.13	0.48
71:1:347:A:C8	71:1:347:A:OP2	2.66	0.48
71:1:991:G:N1	71:1:992:G:C2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:1123:U:O2'	71:1:1124:A:H5'	2.13	0.48
71:1:1126:A:H4'	71:1:1127:U:OP1	2.14	0.48
1:A:86:TYR:HE1	1:A:91:GLU:HG2	1.78	0.48
1:A:166:HIS:HD2	1:A:222:VAL:HG23	1.79	0.48
9:I:187:PHE:CE1	9:I:250:TRP:HB2	2.49	0.48
11:K:21:ARG:NH1	11:K:29:ARG:O	2.34	0.48
13:M:139:VAL:O	13:M:141:SER:N	2.46	0.48
16:P:53:PHE:HB2	16:P:56:ASP:HA	1.95	0.48
17:Q:158:ARG:O	17:Q:162:VAL:HG23	2.14	0.48
19:S:331:ARG:NH1	52:BP:62:GLU:OE1	2.46	0.48
24:X:128:LEU:HB2	24:X:166:ASN:ND2	2.28	0.48
24:X:266:PRO:HA	24:X:285:PHE:HD2	1.79	0.48
25:Y:279:HIS:CD2	25:Y:281:ALA:H	2.32	0.48
52:BP:79:ASP:HB3	52:BP:82:ILE:HD12	1.95	0.48
52:BP:163:ARG:HG3	52:BP:164:ARG:N	2.28	0.48
65:BL:284:ASN:ND2	71:1:671:U:H1'	2.27	0.48
66:BO:60:LEU:HB2	66:BO:86:GLU:HB2	1.95	0.48
71:1:70:G:OP1	71:1:70:G:H4'	2.14	0.48
71:1:448:U:O2'	71:1:449:U:O5'	2.30	0.48
71:1:691:G:C2	71:1:709:U:O2	2.66	0.48
1:A:169:ARG:NH1	1:A:172:ASP:OD2	2.46	0.48
5:E:145:TYR:CG	5:E:190:ALA:HB2	2.48	0.48
6:F:6:LEU:H	6:F:8:ARG:NH1	2.12	0.48
8:H:30:ARG:HH11	71:1:389:A:H62	1.60	0.48
9:I:223:HIS:CE1	54:BF:87:LEU:HG	2.48	0.48
11:K:77:TRP:HZ2	11:K:81:ARG:HH11	1.61	0.48
13:M:31:HIS:CE1	71:1:177:G:H5'	2.47	0.48
13:M:143:TRP:CD1	13:M:229:SER:HB2	2.48	0.48
13:M:204:CYS:HG	13:M:229:SER:HG	1.58	0.48
14:N:150:GLU:HG3	14:N:152:ARG:HH12	1.77	0.48
15:O:218:VAL:O	15:O:226:LEU:HA	2.14	0.48
18:R:289:SER:HA	18:R:476:GLY:O	2.13	0.48
26:Z:76:ARG:HH22	71:1:70:G:P	2.37	0.48
27:BA:15:LEU:C	27:BA:17:LYS:H	2.16	0.48
65:BL:127:LYS:HG3	71:1:667:A:OP1	2.13	0.48
69:UC:103:UNK:O	69:UC:107:UNK:N	2.47	0.48
71:1:162:G:H2'	71:1:162:G:N3	2.28	0.48
71:1:649:A:HO2'	71:1:650:U:P	2.35	0.48
71:1:1068:A:N6	71:1:1096:A:H2'	2.29	0.48
71:1:1079:A:C6	71:1:1080:A:N7	2.82	0.48
1:A:67:TYR:OH	1:A:91:GLU:OE1	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASP:OD1	1:A:246:TYR:N	2.47	0.48
1:A:400:ASP:OD1	1:A:400:ASP:N	2.44	0.48
3:C:112:GLU:HG2	3:C:140:ASN:HA	1.95	0.48
4:D:122:PHE:O	4:D:126:THR:N	2.46	0.48
10:J:53:ILE:HG23	10:J:54:ILE:HG22	1.95	0.48
13:M:82:ARG:HG3	13:M:93:THR:HB	1.94	0.48
27:BA:101:CYS:HA	27:BA:104:LEU:HD12	1.94	0.48
28:UA:186:UNK:O	28:UA:190:UNK:N	2.47	0.48
29:BB:109:THR:O	29:BB:110:PHE:CB	2.62	0.48
37:BC:26:TRP:O	37:BC:30:GLN:HG2	2.14	0.48
44:BM:95:GLU:OE2	44:BM:115:ASN:HB2	2.12	0.48
52:BP:-14:PHE:HE2	52:BP:-9:PRO:HG2	1.78	0.48
71:1:206:U:O2'	71:1:207:G:H5'	2.13	0.48
71:1:361:A:O5'	71:1:361:A:H8	1.96	0.48
71:1:548:A:O2'	71:1:549:C:O5'	2.25	0.48
71:1:941:A:N1	71:1:942:C:N4	2.61	0.48
71:1:1105:G:H8	71:1:1105:G:OP2	1.96	0.48
2:B:194:LYS:HE2	2:B:195:THR:N	2.27	0.48
3:C:26:PRO:HG3	3:C:43:SER:HB3	1.96	0.48
14:N:78:ARG:HH21	14:N:79:ASP:N	2.11	0.48
18:R:48:GLN:HA	18:R:51:TRP:HB3	1.96	0.48
22:V:119:GLN:HE22	22:V:123:LEU:HD21	1.77	0.48
24:X:328:PRO:O	24:X:418:TRP:HD1	1.95	0.48
24:X:363:PHE:HB2	24:X:364:PRO:HD3	1.96	0.48
24:X:421:GLN:OE1	24:X:421:GLN:N	2.45	0.48
25:Y:244:ARG:O	25:Y:248:ASN:ND2	2.47	0.48
27:BA:21:ALA:N	27:BA:22:PRO:HD2	2.28	0.48
27:BA:41:SER:HA	27:BA:44:GLN:NE2	2.27	0.48
44:BM:277:PRO:O	44:BM:281:GLN:NE2	2.29	0.48
65:BL:296:GLU:N	65:BL:296:GLU:OE1	2.47	0.48
71:1:536:A:N6	71:1:861:A:OP1	2.47	0.48
71:1:576:A:OP1	71:1:576:A:H4'	2.14	0.48
71:1:880:A:N6	71:1:881:G:O6	2.46	0.48
71:1:1093:G:C6	71:1:1094:U:C2	3.01	0.48
1:A:364:LEU:HD23	70:UD:36:UNK:HA	1.96	0.48
3:C:71:TYR:H	61:BD:79:GLN:HE22	1.60	0.48
6:F:16:LEU:HD23	6:F:30:ALA:HB2	1.95	0.48
9:I:11:ARG:HH22	66:BO:53:GLY:HA2	1.79	0.48
9:I:38:TRP:HA	9:I:52:ARG:HB3	1.96	0.48
9:I:178:ASP:OD1	9:I:179:TYR:N	2.46	0.48
10:J:77:ASP:HB2	10:J:90:LYS:CB	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:175:ASP:HB3	15:O:190:GLN:HE21	1.78	0.48
20:T:59:PHE:HE1	20:T:66:PRO:HG3	1.78	0.48
24:X:141:ARG:NH2	24:X:163:ALA:O	2.47	0.48
24:X:348:VAL:O	24:X:349:PRO:C	2.51	0.48
25:Y:220:TYR:OH	37:BC:64:GLU:OE2	2.31	0.48
44:BM:68:LEU:HD13	44:BM:72:TYR:CD2	2.49	0.48
65:BL:73:SER:O	65:BL:75:ASP:N	2.45	0.48
65:BL:177:TYR:CG	65:BL:177:TYR:O	2.67	0.48
71:1:1075:A:H2'	71:1:1076:A:O4'	2.14	0.48
1:A:346:GLU:HG2	1:A:347:HIS:N	2.28	0.48
2:B:49:VAL:HG11	2:B:214:GLN:HB2	1.94	0.48
2:B:118:THR:OG1	7:G:84:GLN:OE1	2.20	0.48
2:B:149:LYS:HZ3	2:B:153:ASN:HB2	1.79	0.48
6:F:29:ILE:HG13	6:F:145:TRP:NE1	2.29	0.48
8:H:34:ASP:OD1	8:H:35:PRO:HD2	2.14	0.48
15:O:258:ALA:HB1	15:O:260:GLN:NE2	2.29	0.48
15:O:317:VAL:HG12	17:Q:180:LEU:HD12	1.95	0.48
21:U:68:LEU:N	21:U:85:GLU:HG2	2.28	0.48
54:BF:70:ARG:NE	54:BF:76:SER:OG	2.43	0.48
66:BO:101:VAL:HG22	66:BO:103:VAL:HG12	1.96	0.48
71:1:107:U:H6	71:1:107:U:OP1	1.96	0.48
71:1:145:A:H5"	71:1:146:U:OP2	2.14	0.48
71:1:162:G:H1	71:1:401:U:H6	1.61	0.48
71:1:642:A:H2'	71:1:643:G:O4'	2.13	0.48
71:1:1038:U:H5	71:1:1056:A:C8	2.31	0.48
2:B:120:GLU:HA	2:B:120:GLU:OE2	2.14	0.48
2:B:188:MET:N	2:B:304:LYS:O	2.40	0.48
7:G:185:ASP:OD1	7:G:186:THR:N	2.47	0.48
8:H:134:ASN:H	8:H:137:GLU:HB2	1.79	0.48
9:I:188:LEU:HD22	9:I:258:TRP:CH2	2.49	0.48
10:J:86:LYS:HD2	10:J:86:LYS:HA	1.68	0.48
17:Q:48:ARG:HB3	71:1:100:A:H4'	1.95	0.48
18:R:172:LYS:O	18:R:335:THR:HG22	2.14	0.48
19:S:275:ARG:O	19:S:279:GLU:HG3	2.14	0.48
19:S:281:ARG:HE	52:BP:49:GLN:NE2	2.12	0.48
24:X:263:MET:HG2	24:X:288:ASN:HD22	1.79	0.48
24:X:278:ARG:HG2	24:X:279:HIS:CD2	2.49	0.48
24:X:326:PRO:HB3	24:X:337:HIS:CE1	2.49	0.48
26:Z:48:LYS:HB3	71:1:71:A:H8	1.79	0.48
44:BM:39:VAL:HB	44:BM:108:LEU:HG	1.94	0.48
61:BD:15:ASN:CG	61:BD:68:ARG:HH12	2.18	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BL:158:TRP:HB3	65:BL:176:LEU:HB2	1.96	0.48
65:BL:260:PRO:HB2	71:1:671:U:OP1	2.13	0.48
65:BL:330:LEU:HA	65:BL:335:HIS:H	1.78	0.48
71:1:166:U:H1'	71:1:847:A:H61	1.79	0.48
71:1:390:A:C2	71:1:391:A:C4	3.02	0.48
71:1:548:A:H2'	71:1:588:A:C2	2.45	0.48
71:1:876:G:C2	71:1:991:G:N2	2.82	0.48
71:1:1022:A:N6	71:1:1023:A:N1	2.61	0.48
71:1:1077:G:H2'	71:1:1078:C:C6	2.48	0.48
5:E:295:ARG:NE	5:E:295:ARG:HA	2.29	0.47
6:F:1:MET:HG3	6:F:3:LYS:HG2	1.96	0.47
7:G:237:ALA:HB2	7:G:252:PHE:CE2	2.49	0.47
7:G:285:LEU:HA	7:G:289:ALA:HB3	1.96	0.47
9:I:210:ASP:O	9:I:214:SER:OG	2.14	0.47
10:J:65:ASN:O	10:J:66:PRO:C	2.51	0.47
13:M:81:ASN:ND2	13:M:112:LYS:HG3	2.29	0.47
13:M:250:PRO:HB3	20:T:56:GLU:HB3	1.95	0.47
18:R:290:VAL:HG12	18:R:293:LYS:HD2	1.95	0.47
19:S:244:THR:HA	27:BA:111:ALA:HB2	1.96	0.47
22:V:50:PRO:HA	22:V:53:ARG:NH1	2.29	0.47
24:X:176:ASN:OD1	24:X:180:ARG:NH1	2.47	0.47
24:X:373:LEU:HB3	24:X:374:HIS:CD2	2.49	0.47
27:BA:105:PRO:HG2	27:BA:135:PHE:HE2	1.78	0.47
65:BL:218:THR:H	65:BL:221:LYS:NZ	2.11	0.47
66:BO:42:SER:C	66:BO:44:ARG:H	2.16	0.47
66:BO:134:ARG:NH1	66:BO:148:ASP:O	2.47	0.47
71:1:574:A:O2'	71:1:575:G:H8	1.97	0.47
71:1:752:U:C4	71:1:753:U:C2	3.01	0.47
1:A:394:THR:O	1:A:398:VAL:HG23	2.15	0.47
8:H:61:GLN:HG2	8:H:114:TYR:CE2	2.49	0.47
11:K:114:CYS:SG	11:K:115:ALA:N	2.88	0.47
12:L:39:VAL:HG22	12:L:117:ARG:HD2	1.96	0.47
13:M:41:GLN:NE2	15:O:44:LEU:HD12	2.29	0.47
18:R:18:ASP:OD1	18:R:19:GLY:N	2.47	0.47
21:U:34:ILE:HB	21:U:37:ASN:HB2	1.94	0.47
44:BM:321:LYS:HB3	44:BM:325:GLN:NE2	2.29	0.47
65:BL:86:ASP:OD1	65:BL:87:ILE:N	2.45	0.47
65:BL:119:ARG:NH1	65:BL:132:HIS:CB	2.75	0.47
65:BL:334:ILE:HB	65:BL:336:PRO:CD	2.43	0.47
71:1:649:A:H3'	71:1:1093:G:H21	1.80	0.47
71:1:652:A:H4'	71:1:653:A:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:749:U:C5	71:1:750:U:C4	3.01	0.47
71:1:839:A:N7	71:1:856:A:H2	2.11	0.47
3:C:120:ASN:HB3	3:C:129:TRP:HZ3	1.79	0.47
4:D:124:LEU:HA	4:D:127:LEU:HB2	1.96	0.47
13:M:97:TRP:O	13:M:97:TRP:HE3	1.91	0.47
13:M:98:ALA:HB2	13:M:111:TRP:HD1	1.79	0.47
15:O:311:GLN:NE2	34:BI:250:ALA:HB2	2.30	0.47
44:BM:140:ARG:HG2	44:BM:271:ARG:CZ	2.43	0.47
61:BD:44:TYR:OH	61:BD:48:GLN:NE2	2.47	0.47
66:BO:77:VAL:CB	66:BO:104:GLN:HG3	2.43	0.47
66:BO:101:VAL:O	66:BO:103:VAL:HG13	2.13	0.47
71:1:40:C:H4'	71:1:41:A:H8	1.79	0.47
71:1:131:U:H1'	71:1:132:U:OP1	2.14	0.47
71:1:345:A:H62	71:1:379:U:C5'	2.27	0.47
71:1:408:U:H2'	71:1:409:A:H8	1.80	0.47
71:1:444:A:C1'	71:1:458:A:H8	2.27	0.47
71:1:487:U:O2'	71:1:488:U:OP1	2.28	0.47
71:1:923:A:H1'	71:1:979:G:C8	2.48	0.47
1:A:271:ARG:N	71:1:605:U:OP1	2.47	0.47
7:G:28:VAL:HG13	19:S:322:ILE:HB	1.96	0.47
7:G:69:ARG:HB2	71:1:497:A:H5"	1.97	0.47
9:I:258:TRP:N	9:I:258:TRP:CD1	2.82	0.47
12:L:123:TYR:CZ	12:L:125:PRO:HB3	2.49	0.47
13:M:190:LYS:HD3	13:M:192:LEU:HD23	1.97	0.47
15:O:98:ASP:OD2	54:BF:66:ALA:HB2	2.14	0.47
16:P:35:ILE:O	16:P:38:THR:OG1	2.30	0.47
22:V:66:ARG:H	71:1:967:A:P	2.37	0.47
26:Z:115:PRO:HA	26:Z:118:HIS:CD2	2.49	0.47
27:BA:50:ALA:HA	27:BA:53:LYS:HB2	1.95	0.47
65:BL:324:PRO:HG2	71:1:710:A:OP1	2.14	0.47
66:BO:139:ARG:NH1	66:BO:143:LEU:HD23	2.23	0.47
67:BG:1330:SER:O	67:BG:1333:ILE:HG23	2.15	0.47
71:1:556:A:H5'	71:1:557:A:H5'	1.96	0.47
71:1:924:U:O2'	71:1:925:G:C8	2.58	0.47
2:B:194:LYS:HB3	2:B:194:LYS:HZ3	1.80	0.47
5:E:142:ARG:HG3	5:E:144:ASN:OD1	2.14	0.47
6:F:113:ARG:HD2	71:1:151:G:H5"	1.97	0.47
8:H:61:GLN:HG3	8:H:112:PHE:O	2.14	0.47
17:Q:193:SER:HB3	17:Q:195:GLU:OE1	2.15	0.47
21:U:77:LEU:HD12	21:U:81:THR:HG21	1.97	0.47
22:V:12:ALA:HB3	22:V:17:ILE:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:53:ARG:HE	22:V:109:ARG:NH2	2.11	0.47
26:Z:91:ASN:O	26:Z:95:GLN:HB2	2.13	0.47
28:UA:86:UNK:O	28:UA:88:UNK:N	2.47	0.47
44:BM:119:THR:O	44:BM:121:ARG:N	2.48	0.47
47:BH:69:TYR:CE1	71:1:360:U:C2	3.02	0.47
52:BP:156:ARG:NH2	71:1:420:A:OP2	2.48	0.47
71:1:48:U:N3	71:1:130:U:H5	2.12	0.47
71:1:90:A:H2'	71:1:90:A:N3	2.28	0.47
71:1:143:A:H2'	71:1:144:U:C5	2.50	0.47
71:1:433:G:O2'	71:1:434:U:P	2.73	0.47
71:1:553:A:C2'	71:1:554:G:H5'	2.45	0.47
1:A:182:ALA:HB3	1:A:208:VAL:HG12	1.97	0.47
3:C:123:ASP:OD1	3:C:124:GLU:N	2.48	0.47
5:E:66:PRO:N	5:E:67:PRO:HD2	2.29	0.47
5:E:236:ALA:HB1	5:E:237:PRO:HD2	1.96	0.47
6:F:4:GLN:O	6:F:8:ARG:NH2	2.44	0.47
8:H:30:ARG:O	8:H:115:LYS:NZ	2.42	0.47
16:P:161:ARG:HD2	16:P:181:ARG:HE	1.80	0.47
17:Q:154:GLU:CD	17:Q:157:ARG:HH21	2.17	0.47
17:Q:221:GLU:HA	17:Q:224:LYS:HB2	1.96	0.47
44:BM:247:PHE:HA	44:BM:266:TRP:CH2	2.49	0.47
71:1:52:U:H3'	71:1:53:A:H5"	1.96	0.47
71:1:781:A:H1'	71:1:782:U:OP1	2.13	0.47
71:1:880:A:N1	71:1:987:A:N1	2.63	0.47
1:A:169:ARG:HH22	29:BB:25:LEU:HD22	1.80	0.47
3:C:136:THR:HG21	3:C:172:HIS:HE1	1.80	0.47
4:D:60:PRO:HG2	4:D:62:GLN:HG3	1.96	0.47
5:E:151:LEU:HG	5:E:191:ILE:HD12	1.97	0.47
6:F:57:ILE:HG12	6:F:128:TYR:O	2.14	0.47
6:F:147:ASP:OD1	6:F:148:THR:N	2.48	0.47
7:G:325:THR:OG1	7:G:327:ARG:O	2.29	0.47
8:H:26:ILE:HG23	8:H:28:GLN:HG2	1.96	0.47
8:H:94:VAL:HG12	8:H:94:VAL:O	2.14	0.47
9:I:251:THR:OG1	9:I:252:GLU:OE1	2.31	0.47
10:J:58:ILE:HG13	10:J:58:ILE:O	2.15	0.47
11:K:31:GLU:HG2	15:O:38:LYS:HD3	1.97	0.47
13:M:12:LEU:HD13	13:M:12:LEU:C	2.34	0.47
13:M:37:TRP:CH2	13:M:47:PRO:HG3	2.50	0.47
14:N:196:ARG:HD3	71:1:563:U:OP1	2.15	0.47
16:P:30:LYS:HB3	16:P:48:GLU:O	2.15	0.47
16:P:51:ARG:HG3	16:P:53:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:122:MET:HB3	17:Q:126:ALA:HB3	1.96	0.47
21:U:29:VAL:O	21:U:30:ILE:HB	2.13	0.47
24:X:181:LEU:HD22	24:X:188:LYS:HA	1.96	0.47
24:X:352:LYS:HB3	24:X:353:PRO:CD	2.35	0.47
25:Y:234:ILE:HG13	25:Y:235:MET:N	2.30	0.47
27:BA:113:MET:HG2	27:BA:114:PHE:N	2.27	0.47
27:BA:117:ALA:HB3	27:BA:123:ALA:HB2	1.97	0.47
37:BC:106:ALA:O	37:BC:107:GLU:HG3	2.14	0.47
44:BM:233:VAL:HA	44:BM:236:LEU:HG	1.97	0.47
47:BH:201:GLU:O	47:BH:204:GLN:N	2.48	0.47
47:BH:210:GLU:HG3	47:BH:211:ARG:H	1.79	0.47
47:BH:229:TYR:CD2	52:BP:59:ARG:HD2	2.50	0.47
50:BE:57:THR:HG23	50:BE:58:THR:H	1.78	0.47
61:BD:54:TYR:HB2	61:BD:75:VAL:HG21	1.96	0.47
65:BL:111:SER:OG	65:BL:301:ARG:NH2	2.42	0.47
65:BL:188:THR:HB	65:BL:224:HIS:HE1	1.79	0.47
66:BO:97:VAL:HB	66:BO:99:HIS:HE1	1.80	0.47
71:1:145:A:H3'	71:1:146:U:H5"	1.97	0.47
71:1:1067:C:HO2'	71:1:1068:A:P	2.37	0.47
71:1:1097:A:O2'	71:1:1098:A:P	2.72	0.47
2:B:194:LYS:C	2:B:194:LYS:CE	2.72	0.47
5:E:145:TYR:CD2	5:E:190:ALA:HB2	2.50	0.47
9:I:78:ILE:HD13	9:I:128:ALA:HB2	1.96	0.47
13:M:196:HIS:HB3	13:M:238:ASP:O	2.14	0.47
14:N:169:HIS:CE1	14:N:220:VAL:HG22	2.50	0.47
18:R:207:LYS:NZ	18:R:314:ALA:H	2.12	0.47
19:S:243:THR:O	19:S:245:THR:HG23	2.15	0.47
26:Z:76:ARG:HH21	26:Z:80:ARG:CZ	2.27	0.47
29:BB:17:HIS:CE1	71:1:1118:G:HO2'	2.32	0.47
44:BM:302:MET:HA	44:BM:305:ASP:HB2	1.97	0.47
67:BG:1319:SER:O	67:BG:1323:LEU:HD13	2.15	0.47
71:1:798:A:H2	71:1:799:A:C6	2.33	0.47
71:1:837:U:H2'	71:1:838:A:C8	2.50	0.47
71:1:904:A:H4'	71:1:906:C:OP1	2.14	0.47
2:B:169:ASN:O	2:B:175:GLY:HA3	2.15	0.47
7:G:156:ARG:O	22:V:63:ARG:NH2	2.47	0.47
17:Q:75:VAL:HG23	17:Q:121:PRO:O	2.15	0.47
20:T:31:ARG:HD3	71:1:834:A:N7	2.30	0.47
25:Y:63:ASP:OD1	25:Y:64:VAL:N	2.48	0.47
25:Y:231:GLN:NE2	25:Y:234:ILE:HD11	2.30	0.47
27:BA:52:MET:O	27:BA:56:LEU:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BM:69:LEU:HD11	44:BM:371:TRP:CE3	2.49	0.47
61:BD:13:CYS:SG	61:BD:15:ASN:N	2.82	0.47
66:BO:96:ALA:HB2	66:BO:178:TYR:OH	2.15	0.47
71:1:168:U:H2'	71:1:169:U:C6	2.49	0.47
71:1:423:G:H2'	71:1:423:G:N3	2.30	0.47
71:1:559:U:C2'	71:1:560:U:H5"	2.45	0.47
71:1:1063:U:H4'	71:1:1064:G:N2	2.30	0.47
71:1:1113:G:C5	71:1:1114:A:C2	3.03	0.47
1:A:158:PHE:CZ	1:A:316:ILE:HG21	2.50	0.47
2:B:199:SER:O	2:B:203:LEU:HD12	2.15	0.47
3:C:160:GLU:O	3:C:164:LEU:HG	2.15	0.47
10:J:52:GLN:HE21	10:J:75:VAL:HG21	1.80	0.47
18:R:448:ASP:OD1	18:R:451:CYS:N	2.46	0.47
18:R:455:LYS:CG	71:1:66:U:H3	2.22	0.47
24:X:357:THR:HG23	24:X:358:GLU:N	2.30	0.47
71:1:58:A:C4	71:1:114:A:C2	3.03	0.47
71:1:303:U:HO2'	71:1:304:G:P	2.38	0.47
71:1:862:A:H61	71:1:1105:G:H1	1.63	0.47
71:1:933:G:C2'	71:1:934:G:C8	2.95	0.47
1:A:302:ASP:OD1	1:A:302:ASP:N	2.48	0.46
7:G:42:ALA:HB2	19:S:336:GLN:HB3	1.97	0.46
7:G:110:HIS:CE1	13:M:20:ASN:HB3	2.51	0.46
8:H:11:LEU:HD23	8:H:11:LEU:H	1.80	0.46
8:H:53:THR:O	8:H:119:GLY:N	2.32	0.46
9:I:113:GLN:O	9:I:116:ALA:N	2.48	0.46
10:J:29:ILE:O	10:J:33:LEU:N	2.37	0.46
13:M:17:LYS:HE2	13:M:33:ALA:O	2.14	0.46
13:M:46:ARG:NE	71:1:517:U:O2	2.48	0.46
18:R:146:SER:OG	18:R:147:ARG:N	2.48	0.46
18:R:244:GLU:OE1	18:R:244:GLU:N	2.45	0.46
21:U:18:LEU:CG	21:U:19:LYS:H	2.28	0.46
24:X:502:MET:HA	24:X:508:PRO:HA	1.97	0.46
44:BM:232:ALA:O	44:BM:236:LEU:N	2.45	0.46
44:BM:255:ARG:HB3	44:BM:256:PRO:HD3	1.97	0.46
65:BL:113:ARG:HH22	71:1:289:A:H1'	1.80	0.46
66:BO:101:VAL:O	66:BO:101:VAL:HG13	2.15	0.46
66:BO:136:THR:O	66:BO:136:THR:OG1	2.32	0.46
71:1:442:U:H4'	71:1:443:G:H8	1.80	0.46
71:1:911:A:N1	71:1:912:U:C2	2.82	0.46
3:C:101:GLU:HG2	61:BD:45:HIS:CG	2.50	0.46
8:H:99:GLU:HG3	71:1:390:A:C4	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:149:VAL:O	18:R:58:ARG:NH2	2.44	0.46
16:P:161:ARG:HD2	16:P:181:ARG:HB2	1.98	0.46
24:X:228:GLU:OE1	24:X:228:GLU:N	2.48	0.46
24:X:293:ASN:H	24:X:344:GLN:HE22	1.63	0.46
24:X:328:PRO:HD2	24:X:422:VAL:HG21	1.97	0.46
44:BM:242:THR:H	44:BM:276:HIS:CE1	2.33	0.46
47:BH:168:ILE:O	47:BH:172:VAL:HG23	2.15	0.46
71:1:295:G:N1	71:1:296:U:O2	2.48	0.46
71:1:444:A:HO2'	71:1:458:A:H8	1.60	0.46
1:A:169:ARG:HH22	29:BB:25:LEU:CD2	2.28	0.46
2:B:434:MET:HG3	7:G:275:MET:HB3	1.97	0.46
6:F:84:ARG:HE	6:F:84:ARG:HB3	1.50	0.46
8:H:146:ARG:NH1	52:BP:171:PHE:O	2.48	0.46
9:I:148:ARG:HA	9:I:161:TYR:HA	1.97	0.46
14:N:198:ARG:NH1	71:1:561:U:OP1	2.40	0.46
16:P:49:GLN:NE2	16:P:64:TYR:O	2.48	0.46
25:Y:147:VAL:HG12	25:Y:149:GLN:H	1.80	0.46
28:UA:27:UNK:O	28:UA:31:UNK:N	2.49	0.46
44:BM:125:GLU:O	44:BM:129:LEU:HB2	2.14	0.46
47:BH:80:PRO:HA	47:BH:188:TRP:HA	1.96	0.46
47:BH:80:PRO:HD2	47:BH:98:LYS:HB3	1.97	0.46
47:BH:88:PHE:CG	47:BH:89:VAL:HG13	2.50	0.46
50:BE:65:PHE:HZ	50:BE:67:LYS:HE3	1.78	0.46
65:BL:218:THR:OG1	65:BL:221:LYS:NZ	2.35	0.46
65:BL:310:ARG:O	65:BL:313:SER:N	2.24	0.46
65:BL:358:ARG:NH2	71:1:663:U:OP2	2.48	0.46
66:BO:47:TRP:H	71:1:814:A:H2	1.63	0.46
71:1:47:A:H61	71:1:131:U:H3	1.62	0.46
71:1:171:U:H3	71:1:532:U:H3	1.64	0.46
71:1:343:A:O2'	71:1:344:U:OP1	2.26	0.46
71:1:649:A:H5"	71:1:1075:A:H5'	1.98	0.46
71:1:702:U:H5'	71:1:703:U:OP2	2.15	0.46
71:1:847:A:O2'	71:1:848:U:H5"	2.15	0.46
1:A:40:SER:OG	29:BB:75:VAL:HG22	2.16	0.46
7:G:282:ARG:NH2	7:G:368:ARG:HH12	2.13	0.46
11:K:168:LEU:HD12	11:K:179:TRP:CE3	2.50	0.46
13:M:181:GLU:O	13:M:185:GLN:HB2	2.15	0.46
14:N:122:PRO:HG2	14:N:123:HIS:CE1	2.50	0.46
24:X:242:GLU:O	24:X:245:ASP:HB2	2.15	0.46
29:BB:111:PHE:CD1	29:BB:112:LEU:N	2.83	0.46
37:BC:54:MET:O	37:BC:56:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BP:99:VAL:HG23	52:BP:99:VAL:O	2.16	0.46
65:BL:237:CYS:SG	65:BL:260:PRO:HD3	2.55	0.46
71:1:138:A:H8	71:1:138:A:OP2	1.98	0.46
71:1:426:G:O2'	71:1:427:U:O5'	2.30	0.46
71:1:642:A:HO2'	71:1:643:G:P	2.33	0.46
71:1:880:A:H8	71:1:880:A:O5'	1.97	0.46
1:A:314:SER:O	1:A:314:SER:OG	2.33	0.46
5:E:95:LYS:HB2	5:E:95:LYS:HE3	1.79	0.46
6:F:22:GLN:HA	6:F:61:VAL:O	2.15	0.46
7:G:57:PHE:CD2	52:BP:29:PRO:HD2	2.51	0.46
9:I:98:ASP:HA	9:I:143:TYR:HD2	1.81	0.46
9:I:99:HIS:O	9:I:103:LEU:N	2.48	0.46
11:K:35:GLY:O	11:K:39:ILE:HG22	2.15	0.46
11:K:168:LEU:HD23	11:K:168:LEU:HA	1.84	0.46
13:M:101:GLU:H	13:M:101:GLU:CD	2.19	0.46
14:N:196:ARG:NH2	71:1:562:U:O2'	2.49	0.46
14:N:209:VAL:HG12	18:R:419:GLN:HE21	1.80	0.46
15:O:91:LYS:NZ	71:1:824:A:N1	2.47	0.46
15:O:167:LEU:HD11	15:O:194:PRO:HG3	1.98	0.46
16:P:71:ARG:HD3	16:P:82:THR:HG21	1.97	0.46
24:X:401:GLU:OE1	24:X:402:ARG:NH2	2.49	0.46
24:X:482:PRO:HG2	71:1:203:A:N6	2.30	0.46
26:Z:62:PHE:HZ	26:Z:131:TRP:CH2	2.33	0.46
27:BA:118:SER:OG	27:BA:119:GLU:N	2.48	0.46
37:BC:3:ASP:O	37:BC:6:ALA:N	2.48	0.46
54:BF:23:PRO:O	54:BF:24:LEU:HG	2.15	0.46
65:BL:187:LEU:O	65:BL:279:ALA:HB2	2.16	0.46
65:BL:247:LEU:HD11	65:BL:258:LEU:HB2	1.97	0.46
65:BL:335:HIS:CG	65:BL:335:HIS:O	2.66	0.46
71:1:432:U:N3	71:1:433:G:C6	2.84	0.46
71:1:433:G:O6	71:1:453:A:H2	1.99	0.46
71:1:457:C:H4'	71:1:458:A:OP1	2.15	0.46
71:1:698:G:H2'	71:1:699:A:C5'	2.46	0.46
71:1:855:A:C2	71:1:856:A:C4	3.03	0.46
3:C:100:LEU:HA	3:C:104:GLU:OE1	2.15	0.46
6:F:155:TYR:CD2	6:F:155:TYR:O	2.69	0.46
7:G:331:ALA:N	7:G:335:GLU:OE1	2.25	0.46
9:I:60:ALA:HB3	9:I:66:ARG:HB2	1.98	0.46
9:I:97:ALA:HB3	9:I:144:ALA:HB2	1.97	0.46
11:K:170:ARG:H	11:K:174:ARG:HG3	1.81	0.46
14:N:112:VAL:HG11	18:R:399:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:59:SER:C	16:P:60:ARG:HG3	2.36	0.46
20:T:80:GLN:HG3	20:T:81:ILE:N	2.30	0.46
25:Y:253:PHE:O	25:Y:257:GLU:N	2.36	0.46
26:Z:43:ILE:O	26:Z:43:ILE:HG22	2.16	0.46
27:BA:113:MET:O	27:BA:114:PHE:CG	2.68	0.46
37:BC:132:ILE:O	37:BC:132:ILE:HG13	2.16	0.46
44:BM:253:CYS:HB3	44:BM:259:LYS:HB2	1.97	0.46
61:BD:50:ARG:HG2	61:BD:54:TYR:CE1	2.49	0.46
71:1:249:U:O2	71:1:249:U:O5'	2.34	0.46
71:1:764:U:O2'	71:1:765:A:OP1	2.33	0.46
71:1:869:A:O2'	71:1:870:A:P	2.73	0.46
71:1:935:G:C2	71:1:936:G:C4	3.04	0.46
71:1:1045:U:H3'	71:1:1045:U:O2	2.16	0.46
2:B:38:PHE:HB2	7:G:96:TYR:OH	2.16	0.46
2:B:417:VAL:HG23	2:B:418:GLU:OE1	2.15	0.46
5:E:176:ARG:O	5:E:179:ARG:HB3	2.16	0.46
5:E:254:GLN:O	5:E:258:GLY:N	2.47	0.46
6:F:80:GLY:N	71:1:1027:G:H5"	2.30	0.46
13:M:50:ILE:HD11	15:O:54:LEU:HD23	1.98	0.46
14:N:149:VAL:HG21	14:N:182:TYR:CE1	2.51	0.46
15:O:77:ASP:OD2	15:O:79:GLU:HB2	2.16	0.46
16:P:167:TYR:CD1	16:P:172:LEU:HD12	2.51	0.46
17:Q:217:LYS:O	17:Q:221:GLU:HB2	2.16	0.46
18:R:421:ASN:ND2	18:R:448:ASP:HB3	2.31	0.46
18:R:423:SER:OG	18:R:424:ASN:N	2.49	0.46
18:R:479:ASP:OD1	18:R:480:ILE:N	2.49	0.46
20:T:34:ASN:OD1	20:T:34:ASN:N	2.48	0.46
22:V:32:PHE:O	22:V:98:LYS:NZ	2.40	0.46
25:Y:168:GLU:HB2	25:Y:177:PHE:CD1	2.50	0.46
44:BM:75:VAL:CG1	44:BM:79:ARG:HE	2.28	0.46
44:BM:153:HIS:HA	44:BM:156:LEU:HB3	1.97	0.46
44:BM:290:HIS:HB3	44:BM:326:TYR:CE1	2.51	0.46
44:BM:357:ALA:O	44:BM:361:LEU:HD12	2.15	0.46
44:BM:374:LEU:HD12	44:BM:374:LEU:HA	1.82	0.46
52:BP:-10:ARG:HA	52:BP:-10:ARG:HD2	1.75	0.46
52:BP:11:GLY:HA2	52:BP:16:SER:OG	2.16	0.46
61:BD:86:LEU:HA	61:BD:93:ARG:HH21	1.81	0.46
65:BL:183:VAL:HG23	65:BL:183:VAL:O	2.15	0.46
71:1:219:A:C8	71:1:319:A:N6	2.84	0.46
71:1:288:C:O2'	71:1:289:A:O5'	2.33	0.46
71:1:511:A:O2'	71:1:512:A:OP2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:540:U:H5	71:1:541:U:C2	2.34	0.46
71:1:881:G:H8	71:1:987:A:C2	2.33	0.46
71:1:1036:U:H5'	71:1:1037:C:OP1	2.15	0.46
2:B:144:ARG:HD3	14:N:76:TYR:HE1	1.80	0.46
2:B:389:GLU:O	2:B:392:MET:HG2	2.15	0.46
5:E:250:LEU:HB2	5:E:255:LEU:HD13	1.98	0.46
6:F:33:TYR:CZ	6:F:143:LEU:HD11	2.51	0.46
8:H:6:LEU:CG	8:H:7:ARG:H	2.28	0.46
14:N:168:PHE:HE1	14:N:223:VAL:HG11	1.80	0.46
19:S:362:ARG:O	19:S:365:ARG:N	2.49	0.46
22:V:64:ARG:HD3	71:1:955:U:OP2	2.15	0.46
24:X:90:ASP:HB2	24:X:147:TYR:CE1	2.51	0.46
26:Z:90:LEU:O	26:Z:94:ILE:HG12	2.16	0.46
28:UA:55:UNK:O	28:UA:59:UNK:N	2.49	0.46
37:BC:16:HIS:HA	37:BC:19:MET:HE2	1.97	0.46
44:BM:67:GLU:HA	44:BM:323:ARG:NH1	2.31	0.46
66:BO:87:ARG:HG2	66:BO:88:PHE:H	1.80	0.46
66:BO:180:LEU:HD11	66:BO:185:LEU:HD23	1.98	0.46
71:1:599:U:O2'	71:1:600:A:H5'	2.16	0.46
1:A:240:THR:HG21	71:1:1156:U:O4	2.16	0.46
2:B:5:ARG:HB3	2:B:5:ARG:CZ	2.45	0.46
3:C:159:GLU:OE2	3:C:171:ASN:HA	2.16	0.46
3:C:162:TYR:OH	3:C:172:HIS:NE2	2.26	0.46
5:E:92:PRO:HG2	5:E:93:HIS:CE1	2.51	0.46
5:E:148:TYR:CD2	5:E:192:ILE:HD11	2.50	0.46
5:E:202:VAL:HG22	5:E:204:GLY:N	2.25	0.46
9:I:83:VAL:HG23	54:BF:10:ASN:OD1	2.16	0.46
12:L:24:VAL:HA	12:L:32:TYR:O	2.16	0.46
15:O:217:LYS:HD2	15:O:226:LEU:O	2.15	0.46
16:P:47:LYS:NZ	71:1:940:U:O4	2.42	0.46
27:BA:54:LYS:HE3	27:BA:54:LYS:HB2	1.64	0.46
28:UA:136:UNK:O	28:UA:140:UNK:N	2.49	0.46
37:BC:51:ARG:HG3	37:BC:51:ARG:O	2.16	0.46
44:BM:204:THR:HA	44:BM:286:TYR:CE1	2.51	0.46
44:BM:250:GLU:HA	44:BM:265:LEU:O	2.16	0.46
47:BH:215:VAL:CG1	71:1:361:A:H5'	2.46	0.46
52:BP:-3:HIS:O	52:BP:1:MET:N	2.49	0.46
71:1:316:A:H3'	71:1:317:A:H5'	1.98	0.46
71:1:911:A:C2	71:1:912:U:C2	3.04	0.46
1:A:395:GLN:HA	1:A:398:VAL:HB	1.98	0.46
3:C:118:LEU:HD11	3:C:155:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:86:PHE:CE2	5:E:90:THR:HG21	2.51	0.46
8:H:22:THR:HG22	8:H:24:ARG:HD3	1.97	0.46
9:I:217:LYS:HD3	9:I:258:TRP:CZ3	2.51	0.46
9:I:236:GLY:HA3	15:O:94:ASP:O	2.16	0.46
13:M:183:ALA:O	13:M:187:ALA:N	2.48	0.46
15:O:64:LEU:HA	15:O:64:LEU:HD23	1.72	0.46
17:Q:74:ASP:HB3	17:Q:152:TYR:CZ	2.51	0.46
17:Q:192:THR:OG1	17:Q:193:SER:N	2.48	0.46
20:T:69:GLN:HG2	20:T:70:GLY:N	2.31	0.46
23:W:64:VAL:HB	23:W:65:PRO:HD3	1.98	0.46
24:X:254:ALA:HB3	24:X:257:ASN:ND2	2.30	0.46
44:BM:79:ARG:HH21	44:BM:382:LEU:HD13	1.80	0.46
54:BF:58:SER:H	54:BF:95:ASN:HD22	1.64	0.46
65:BL:135:ARG:HG2	65:BL:136:ASP:N	2.30	0.46
65:BL:192:LEU:N	65:BL:197:TYR:OH	2.45	0.46
66:BO:62:ASP:HB2	71:1:617:G:H8	1.81	0.46
71:1:212:A:O2'	71:1:213:U:H5'	2.15	0.46
71:1:565:U:H4'	71:1:566:G:OP1	2.16	0.46
71:1:750:U:H4'	71:1:751:A:H8	1.81	0.46
71:1:1130:A:N6	71:1:1131:A:N1	2.64	0.46
1:A:128:SER:HB3	1:A:353:PHE:HE1	1.81	0.45
2:B:72:HIS:CD2	2:B:74:GLN:HE21	2.34	0.45
2:B:166:ASP:OD1	2:B:168:LYS:HG2	2.17	0.45
3:C:161:ALA:O	3:C:165:LEU:HD23	2.16	0.45
5:E:92:PRO:HG2	5:E:93:HIS:ND1	2.31	0.45
6:F:37:GLN:HG2	6:F:42:PHE:CE2	2.50	0.45
7:G:310:HIS:CD2	7:G:312:GLY:H	2.35	0.45
9:I:173:ASN:HB2	9:I:174:HIS:CD2	2.50	0.45
13:M:131:GLN:O	13:M:190:LYS:NZ	2.42	0.45
15:O:20:THR:OG1	15:O:21:TYR:N	2.48	0.45
15:O:160:VAL:HG13	15:O:165:GLU:HB3	1.99	0.45
15:O:216:VAL:HG23	18:R:283:ILE:HD12	1.98	0.45
16:P:162:PHE:O	25:Y:204:ARG:HD3	2.16	0.45
17:Q:193:SER:HB2	17:Q:196:GLU:CB	2.45	0.45
18:R:153:ARG:NH2	18:R:354:ASP:OD2	2.24	0.45
25:Y:119:ASN:OD1	25:Y:121:GLU:HG2	2.17	0.45
25:Y:209:LEU:HD12	25:Y:214:GLY:HA2	1.98	0.45
27:BA:27:GLY:O	27:BA:29:ALA:N	2.48	0.45
44:BM:290:HIS:HB3	44:BM:326:TYR:HE1	1.81	0.45
44:BM:302:MET:N	44:BM:303:PRO:HD2	2.31	0.45
50:BE:63:GLY:C	50:BE:65:PHE:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:BD:2:SER:HA	61:BD:27:GLN:O	2.16	0.45
65:BL:339:CYS:HB2	71:1:693:A:O2'	2.17	0.45
71:1:121:U:C4	71:1:122:U:N3	2.84	0.45
71:1:125:A:H2'	71:1:126:U:H5'	1.97	0.45
71:1:328:A:H4'	71:1:328:A:OP1	2.15	0.45
71:1:378:A:O2'	71:1:379:U:H5"	2.15	0.45
71:1:439:A:N6	71:1:442:U:OP2	2.50	0.45
71:1:753:U:C4	71:1:754:A:N6	2.84	0.45
71:1:765:A:C6	71:1:766:A:N1	2.83	0.45
71:1:901:G:N2	71:1:908:U:H3	2.09	0.45
71:1:1000:A:H2'	71:1:1001:G:H8	1.81	0.45
1:A:254:ARG:HE	1:A:292:GLY:HA3	1.81	0.45
3:C:114:PRO:HB3	3:C:138:TYR:CE1	2.51	0.45
6:F:131:SER:O	6:F:133:HIS:ND1	2.37	0.45
12:L:42:VAL:HG23	12:L:114:THR:HG23	1.97	0.45
13:M:52:LYS:NZ	71:1:125:A:OP2	2.43	0.45
20:T:67:LYS:HG2	20:T:68:LYS:O	2.16	0.45
21:U:67:LYS:HE3	21:U:84:LYS:NZ	2.32	0.45
24:X:147:TYR:CB	24:X:209:CYS:HB3	2.47	0.45
24:X:286:PHE:HD1	24:X:369:SER:HA	1.80	0.45
29:BB:111:PHE:HD1	29:BB:111:PHE:O	1.99	0.45
34:BI:152:HIS:O	34:BI:254:PRO:HD3	2.17	0.45
34:BI:164:ASP:N	34:BI:164:ASP:OD1	2.48	0.45
37:BC:16:HIS:O	37:BC:19:MET:N	2.49	0.45
66:BO:134:ARG:HD3	71:1:614:A:OP1	2.16	0.45
71:1:48:U:H3	71:1:130:U:H5	1.64	0.45
71:1:204:U:O2'	71:1:205:U:H5"	2.16	0.45
71:1:249:U:O2	71:1:249:U:O4'	2.32	0.45
71:1:338:A:N6	71:1:381:A:C4	2.85	0.45
71:1:961:A:C8	71:1:966:A:N7	2.84	0.45
71:1:1121:U:O2'	71:1:1122:A:O5'	2.29	0.45
1:A:188:GLU:OE2	13:M:258:LYS:NZ	2.36	0.45
2:B:144:ARG:HD3	14:N:76:TYR:CE1	2.52	0.45
8:H:32:TYR:CD2	8:H:91:PHE:HE1	2.34	0.45
8:H:80:PHE:CZ	8:H:133:LEU:HG	2.51	0.45
8:H:149:ILE:HG22	8:H:151:LEU:HD23	1.99	0.45
14:N:78:ARG:NH2	14:N:79:ASP:O	2.49	0.45
16:P:87:MET:SD	16:P:88:THR:N	2.89	0.45
21:U:50:MET:HG2	21:U:92:PHE:CE2	2.52	0.45
22:V:43:ARG:NH2	71:1:956:A:O2'	2.49	0.45
71:1:228:G:H2'	71:1:291:A:N6	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:312:A:H2'	71:1:313:A:O4'	2.16	0.45
71:1:876:G:H3'	71:1:877:G:C8	2.51	0.45
71:1:886:A:C2	71:1:980:A:C5	3.05	0.45
71:1:1022:A:H8	71:1:1022:A:O5'	2.00	0.45
71:1:1075:A:H3'	71:1:1075:A:OP2	2.16	0.45
1:A:35:TYR:C	1:A:37:CYS:H	2.20	0.45
2:B:194:LYS:NZ	71:1:186:U:OP2	2.41	0.45
7:G:79:TRP:HD1	7:G:96:TYR:CD2	2.35	0.45
8:H:35:PRO:HD3	8:H:115:LYS:HD3	1.99	0.45
8:H:135:GLN:HG3	8:H:139:GLU:OE2	2.16	0.45
9:I:152:ARG:HH11	9:I:157:ASN:HB3	1.80	0.45
9:I:263:LEU:O	9:I:266:THR:OG1	2.29	0.45
11:K:108:ARG:NH2	11:K:112:GLU:OE2	2.50	0.45
13:M:9:ASN:HD21	13:M:12:LEU:HD12	1.82	0.45
13:M:259:ARG:NH2	70:UD:15:UNK:HA	2.32	0.45
14:N:112:VAL:HG22	18:R:397:PRO:HB2	1.98	0.45
16:P:52:ARG:O	16:P:54:GLY:N	2.49	0.45
18:R:126:PRO:HB3	34:BI:173:GLN:HE21	1.82	0.45
18:R:311:PHE:CD2	18:R:317:VAL:HG22	2.51	0.45
18:R:393:LEU:HD23	18:R:393:LEU:HA	1.71	0.45
20:T:32:LYS:HG3	71:1:533:U:H1'	1.98	0.45
25:Y:177:PHE:O	25:Y:180:VAL:HG13	2.16	0.45
26:Z:50:PRO:CD	26:Z:53:MET:HE3	2.47	0.45
34:BI:145:THR:O	34:BI:165:ILE:HD12	2.16	0.45
67:BG:1327:LYS:O	67:BG:1331:GLY:HA3	2.16	0.45
71:1:71:A:C2	71:1:72:U:H1'	2.51	0.45
71:1:435:A:OP1	71:1:443:G:H4'	2.17	0.45
71:1:448:U:HO2'	71:1:449:U:H6	1.60	0.45
71:1:844:A:O2'	71:1:845:A:OP1	2.29	0.45
71:1:1001:G:H2'	71:1:1001:G:N3	2.31	0.45
71:1:1049:A:N6	71:1:1050:A:C6	2.85	0.45
2:B:401:TYR:C	2:B:403:PRO:HD3	2.37	0.45
3:C:145:ARG:HH12	17:Q:108:ILE:HG22	1.81	0.45
7:G:138:ALA:HB2	71:1:346:A:C2	2.51	0.45
7:G:165:ARG:HG2	71:1:93:U:OP1	2.16	0.45
8:H:163:GLU:HB2	8:H:167:PHE:CE2	2.51	0.45
9:I:88:ALA:N	71:1:600:A:OP1	2.38	0.45
9:I:114:GLN:HG3	68:UB:21:UNK:CB	2.46	0.45
11:K:187:ASP:OD1	11:K:188:LEU:N	2.49	0.45
13:M:72:LEU:HD22	71:1:50:A:N7	2.31	0.45
13:M:179:ALA:O	13:M:182:VAL:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:178:ILE:HD12	15:O:187:GLN:HG3	1.98	0.45
17:Q:67:PRO:HD3	17:Q:77:TRP:CZ3	2.51	0.45
17:Q:156:ILE:O	17:Q:160:LEU:HB2	2.16	0.45
18:R:153:ARG:O	18:R:156:GLU:HG2	2.17	0.45
19:S:291:VAL:HG21	19:S:301:ILE:HD11	1.98	0.45
20:T:29:PRO:HD2	71:1:830:A:N1	2.32	0.45
22:V:127:GLU:OE1	22:V:127:GLU:N	2.50	0.45
24:X:111:ASP:N	24:X:111:ASP:OD1	2.45	0.45
28:UA:86:UNK:C	28:UA:88:UNK:N	2.79	0.45
34:BI:183:ALA:HB3	34:BI:186:GLU:HB2	1.98	0.45
47:BH:188:TRP:CG	47:BH:227:PRO:HB3	2.51	0.45
65:BL:335:HIS:HD2	65:BL:337:ARG:HH21	1.64	0.45
71:1:383:A:H8	71:1:383:A:O5'	2.00	0.45
71:1:552:A:N1	71:1:584:U:N3	2.64	0.45
3:C:88:THR:HG21	17:Q:61:SER:OG	2.16	0.45
6:F:111:PHE:O	6:F:118:ARG:HG2	2.17	0.45
8:H:60:THR:HG1	8:H:63:GLN:H	1.58	0.45
9:I:61:ARG:H	9:I:65:HIS:CD2	2.23	0.45
9:I:186:PHE:CD1	9:I:186:PHE:C	2.90	0.45
12:L:74:LEU:HD23	12:L:74:LEU:HA	1.74	0.45
13:M:184:GLN:HA	13:M:187:ALA:HB3	1.97	0.45
15:O:296:HIS:CE1	15:O:300:LYS:HD2	2.51	0.45
16:P:62:PRO:HB3	16:P:77:PHE:HD2	1.82	0.45
17:Q:35:ILE:CD1	61:BD:29:ILE:HD12	2.46	0.45
18:R:421:ASN:HD22	18:R:448:ASP:HB3	1.80	0.45
25:Y:181:ASP:OD1	25:Y:182:THR:N	2.49	0.45
26:Z:47:ASN:OD1	26:Z:47:ASN:N	2.50	0.45
50:BE:91:ILE:HG23	50:BE:113:HIS:HE2	1.81	0.45
52:BP:66:LEU:HD23	52:BP:66:LEU:HA	1.74	0.45
52:BP:143:PRO:O	52:BP:147:VAL:HB	2.16	0.45
65:BL:364:ASP:O	65:BL:367:SER:OG	2.34	0.45
71:1:255:U:C4	71:1:279:U:C5	3.05	0.45
71:1:341:U:H4'	71:1:973:U:C6	2.52	0.45
71:1:452:A:C2	71:1:453:A:H1'	2.52	0.45
71:1:553:A:N1	71:1:573:A:H5'	2.32	0.45
71:1:991:G:H2'	71:1:991:G:N3	2.32	0.45
2:B:19:ASP:OD1	2:B:20:PHE:N	2.49	0.45
4:D:90:GLY:O	4:D:93:ARG:HG2	2.17	0.45
7:G:51:TYR:CE2	52:BP:34:GLY:HA2	2.52	0.45
11:K:59:ARG:HA	11:K:62:VAL:HG12	1.99	0.45
16:P:177:ARG:HD3	16:P:177:ARG:HA	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:348:ALA:HA	71:1:368:U:C5	2.52	0.45
44:BM:66:PRO:HD2	44:BM:319:ALA:HB3	1.99	0.45
44:BM:76:TYR:HH	44:BM:326:TYR:HB3	1.82	0.45
44:BM:133:LYS:HA	44:BM:133:LYS:HD3	1.76	0.45
47:BH:70:GLY:H	47:BH:74:LEU:HD13	1.81	0.45
52:BP:97:ARG:CB	52:BP:97:ARG:HH21	2.29	0.45
65:BL:114:ASP:O	65:BL:114:ASP:OD1	2.34	0.45
65:BL:186:LEU:CD2	65:BL:278:ARG:HH11	2.30	0.45
65:BL:352:ARG:NH2	65:BL:357:ASN:OD1	2.49	0.45
71:1:257:G:H2'	71:1:257:G:N3	2.30	0.45
71:1:1130:A:C6	71:1:1131:A:N1	2.85	0.45
1:A:60:HIS:NE2	1:A:65:SER:HB3	2.32	0.45
2:B:399:ASN:ND2	2:B:402:HIS:HB2	2.32	0.45
4:D:32:ARG:HG2	4:D:38:HIS:CE1	2.52	0.45
7:G:341:HIS:HA	7:G:344:LYS:HE2	1.98	0.45
9:I:214:SER:HB3	54:BF:29:ARG:HB2	1.99	0.45
9:I:214:SER:CB	54:BF:29:ARG:HB2	2.47	0.45
10:J:83:THR:O	10:J:83:THR:HG22	2.17	0.45
13:M:41:GLN:HE21	15:O:44:LEU:HD12	1.81	0.45
15:O:19:PHE:O	20:T:52:LEU:HD13	2.16	0.45
17:Q:74:ASP:HB3	17:Q:152:TYR:CE2	2.52	0.45
17:Q:171:PHE:O	17:Q:174:ASP:N	2.49	0.45
18:R:259:VAL:O	18:R:259:VAL:HG23	2.17	0.45
19:S:258:PHE:HE1	19:S:312:GLN:HB2	1.82	0.45
21:U:28:LYS:HZ3	21:U:28:LYS:HB2	1.81	0.45
22:V:139:ALA:HB1	22:V:140:PRO:HD2	1.99	0.45
27:BA:53:LYS:O	27:BA:56:LEU:HB3	2.17	0.45
44:BM:192:LEU:O	44:BM:192:LEU:HD12	2.17	0.45
44:BM:269:VAL:O	44:BM:273:VAL:HG22	2.17	0.45
44:BM:285:LEU:HB3	44:BM:289:ARG:NE	2.30	0.45
52:BP:146:PHE:CD2	52:BP:147:VAL:HG23	2.52	0.45
66:BO:103:VAL:HB	66:BO:105:ARG:CB	2.46	0.45
66:BO:130:LEU:HD12	66:BO:151:THR:O	2.17	0.45
71:1:269:A:H2'	71:1:270:A:H5"	1.98	0.45
71:1:577:A:H2'	71:1:577:A:N3	2.30	0.45
71:1:777:G:H2'	71:1:778:A:C8	2.52	0.45
71:1:1079:A:N6	71:1:1088:G:H1	2.14	0.45
1:A:163:ILE:HG21	1:A:166:HIS:CE1	2.52	0.45
2:B:170:HIS:HE1	71:1:216:U:H4'	1.81	0.45
14:N:138:PHE:HE1	18:R:98:VAL:HG12	1.82	0.45
15:O:161:LYS:HB3	18:R:441:TRP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:231:PRO:HB3	24:X:257:ASN:HD21	1.82	0.45
29:BB:129:THR:HG23	29:BB:130:LYS:HA	1.99	0.45
44:BM:321:LYS:O	44:BM:325:GLN:N	2.40	0.45
54:BF:63:ARG:HH12	54:BF:68:GLN:HA	1.82	0.45
65:BL:119:ARG:HH12	65:BL:132:HIS:HB3	1.81	0.45
66:BO:79:LEU:O	66:BO:79:LEU:HD23	2.16	0.45
66:BO:103:VAL:CB	66:BO:105:ARG:HB3	2.47	0.45
66:BO:103:VAL:CG1	66:BO:122:PRO:HA	2.39	0.45
71:1:143:A:C8	71:1:144:U:H5	2.35	0.45
71:1:976:A:O2'	71:1:977:U:O2	2.29	0.45
3:C:101:GLU:OE1	3:C:101:GLU:N	2.50	0.45
5:E:332:ALA:C	5:E:334:SER:N	2.70	0.45
10:J:45:PRO:HA	10:J:83:THR:HG23	1.99	0.45
15:O:265:GLU:HB2	18:R:41:ARG:NH2	2.31	0.45
16:P:30:LYS:O	71:1:940:U:N3	2.33	0.45
16:P:51:ARG:NE	16:P:53:PHE:HE2	2.15	0.45
18:R:203:GLU:HG2	18:R:207:LYS:HD2	1.98	0.45
20:T:76:GLU:O	20:T:80:GLN:HG2	2.16	0.45
21:U:17:ARG:N	21:U:17:ARG:CD	2.64	0.45
23:W:84:THR:HG22	23:W:102:TRP:HB3	1.99	0.45
24:X:266:PRO:HD3	24:X:338:LEU:HD13	1.99	0.45
28:UA:65:UNK:HA	28:UA:114:UNK:HA	1.97	0.45
29:BB:127:PRO:O	50:BE:43:GLU:HA	2.16	0.45
44:BM:140:ARG:HH12	44:BM:263:ARG:CD	2.30	0.45
47:BH:94:ASP:OD2	47:BH:101:ARG:N	2.49	0.45
54:BF:27:ARG:O	54:BF:27:ARG:HD2	2.16	0.45
54:BF:109:ASP:N	54:BF:109:ASP:OD1	2.50	0.45
66:BO:50:GLY:O	66:BO:52:GLU:HG3	2.16	0.45
71:1:216:U:O4	71:1:217:A:N6	2.50	0.45
71:1:316:A:H3'	71:1:317:A:C5'	2.47	0.45
71:1:480:A:H8	71:1:481:U:H5'	1.82	0.45
71:1:558:C:C4	71:1:559:U:C4	3.05	0.45
71:1:563:U:O2'	71:1:564:U:O4'	2.24	0.45
71:1:762:A:H8	71:1:762:A:O5'	2.00	0.45
71:1:1027:G:H2'	71:1:1028:U:O4'	2.16	0.45
71:1:1141:A:H2'	71:1:1142:U:O4'	2.17	0.45
2:B:91:VAL:HG12	2:B:104:THR:OG1	2.16	0.44
7:G:165:ARG:HA	7:G:169:LYS:HD2	1.99	0.44
9:I:153:ARG:HG3	9:I:160:MET:SD	2.57	0.44
9:I:215:LYS:O	9:I:218:THR:OG1	2.35	0.44
12:L:93:VAL:HG11	12:L:106:TRP:CH2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:26:MET:O	15:O:27:TYR:C	2.54	0.44
17:Q:133:ASP:OD1	17:Q:142:LYS:HD3	2.17	0.44
18:R:131:PRO:HG2	18:R:134:ALA:HB2	1.98	0.44
21:U:49:HIS:CE1	21:U:75:PRO:HG2	2.52	0.44
22:V:64:ARG:CZ	71:1:969:U:C4	3.00	0.44
34:BI:144:LEU:HD11	34:BI:176:ILE:HD13	1.98	0.44
44:BM:47:LYS:HA	44:BM:47:LYS:HD2	1.77	0.44
44:BM:202:SER:OG	44:BM:205:LYS:HE2	2.17	0.44
44:BM:294:ASP:HB3	44:BM:323:ARG:CG	2.46	0.44
65:BL:241:GLY:HA3	71:1:671:U:O4	2.16	0.44
66:BO:51:THR:HG23	66:BO:136:THR:HG21	1.99	0.44
66:BO:80:ILE:HG21	66:BO:100:ARG:HH11	1.80	0.44
71:1:149:U:O2'	71:1:150:A:C8	2.65	0.44
71:1:347:A:H5'	71:1:348:U:OP2	2.17	0.44
2:B:97:LEU:HD23	2:B:97:LEU:HA	1.70	0.44
5:E:103:ARG:CZ	71:1:431:A:H5"	2.46	0.44
5:E:107:TYR:CE2	5:E:113:ILE:HD12	2.45	0.44
7:G:196:THR:N	7:G:199:HIS:HD2	2.15	0.44
7:G:228:TYR:HE1	7:G:230:LEU:HD13	1.82	0.44
13:M:146:LEU:HD23	13:M:204:CYS:SG	2.57	0.44
19:S:377:LYS:HD2	19:S:377:LYS:HA	1.72	0.44
21:U:42:ARG:HA	21:U:50:MET:HA	1.99	0.44
27:BA:107:ASN:HB3	27:BA:110:ARG:HB2	1.98	0.44
65:BL:93:VAL:HG22	65:BL:97:MET:HB2	1.99	0.44
66:BO:60:LEU:HG	66:BO:133:ARG:HH12	1.81	0.44
71:1:372:A:N6	71:1:373:A:C6	2.85	0.44
71:1:447:A:C6	71:1:448:U:C4	3.06	0.44
71:1:508:G:O2'	71:1:509:U:P	2.74	0.44
71:1:572:A:H8	71:1:572:A:H5"	1.83	0.44
71:1:687:U:H2'	71:1:688:C:H5'	1.99	0.44
71:1:812:A:C3'	71:1:813:U:H5'	2.43	0.44
71:1:841:A:N1	71:1:854:A:N1	2.66	0.44
71:1:845:A:H2'	71:1:846:A:H5"	1.98	0.44
71:1:1025:G:H4'	71:1:1025:G:OP1	2.17	0.44
1:A:360:GLU:N	1:A:360:GLU:OE1	2.50	0.44
2:B:80:VAL:HG13	2:B:361:PHE:CE2	2.52	0.44
2:B:250:MET:HG2	2:B:279:VAL:CG2	2.48	0.44
7:G:41:LEU:HD12	7:G:42:ALA:H	1.83	0.44
7:G:217:VAL:HG21	71:1:200:U:O4	2.17	0.44
9:I:90:ALA:HB3	9:I:91:PRO:HD3	2.00	0.44
10:J:52:GLN:HE22	10:J:75:VAL:HG11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:23:GLN:HA	15:O:23:GLN:HE21	1.76	0.44
18:R:208:TRP:CD1	18:R:211:SER:OG	2.69	0.44
24:X:354:MET:O	24:X:355:THR:HB	2.16	0.44
24:X:363:PHE:CB	24:X:364:PRO:HD3	2.48	0.44
44:BM:36:VAL:O	44:BM:122:LEU:HD23	2.17	0.44
47:BH:42:ARG:HE	47:BH:42:ARG:HB2	1.66	0.44
47:BH:215:VAL:HG11	71:1:361:A:H5'	1.98	0.44
65:BL:333:ARG:O	65:BL:334:ILE:HG23	2.17	0.44
71:1:288:C:H1'	71:1:289:A:H5'	1.98	0.44
71:1:543:U:H2'	71:1:598:U:OP1	2.17	0.44
71:1:688:C:H42	71:1:710:A:H62	1.65	0.44
2:B:350:PRO:HB3	7:G:186:THR:HG23	1.98	0.44
3:C:73:MET:O	3:C:82:ASP:HB2	2.17	0.44
3:C:149:LEU:HD11	3:C:156:TYR:CZ	2.51	0.44
5:E:86:PHE:O	5:E:90:THR:HG22	2.16	0.44
5:E:118:PRO:HG3	5:E:165:TRP:HE1	1.83	0.44
7:G:155:PRO:HD3	22:V:59:GLY:O	2.17	0.44
8:H:72:LEU:HD23	8:H:72:LEU:HA	1.79	0.44
9:I:77:LEU:HD22	9:I:93:LEU:HD21	1.99	0.44
9:I:154:ARG:O	15:O:89:HIS:NE2	2.51	0.44
10:J:21:PHE:CD2	10:J:26:ILE:HD11	2.52	0.44
11:K:152:LEU:HD23	11:K:180:MET:HE3	1.99	0.44
19:S:245:THR:HB	27:BA:65:GLY:O	2.18	0.44
21:U:61:LEU:O	21:U:63:ALA:N	2.47	0.44
25:Y:147:VAL:HG11	25:Y:150:LEU:HD13	1.99	0.44
27:BA:123:ALA:HB1	27:BA:140:ALA:O	2.17	0.44
28:UA:111:UNK:O	28:UA:113:UNK:N	2.50	0.44
34:BI:90:SER:O	34:BI:90:SER:OG	2.34	0.44
44:BM:140:ARG:HD2	44:BM:140:ARG:O	2.17	0.44
52:BP:173:VAL:C	52:BP:175:MET:H	2.20	0.44
65:BL:188:THR:HB	65:BL:224:HIS:CE1	2.53	0.44
65:BL:192:LEU:O	65:BL:197:TYR:OH	2.24	0.44
65:BL:339:CYS:O	65:BL:341:LYS:N	2.50	0.44
66:BO:88:PHE:C	66:BO:91:CYS:H	2.21	0.44
71:1:654:A:O5'	71:1:654:A:H8	2.01	0.44
71:1:777:G:H8	71:1:777:G:O5'	2.00	0.44
71:1:924:U:C2	71:1:925:G:C8	3.05	0.44
71:1:1018:A:H61	71:1:1096:A:H2	1.65	0.44
1:A:162:GLN:NE2	1:A:225:LYS:HG2	2.31	0.44
5:E:39:PHE:O	5:E:165:TRP:HB3	2.17	0.44
6:F:49:GLY:H	6:F:124:LYS:NZ	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:139:LYS:HB3	7:G:139:LYS:HE3	1.81	0.44
7:G:197:LEU:HD22	7:G:266:LEU:HD21	2.00	0.44
9:I:89:ARG:O	9:I:93:LEU:N	2.50	0.44
14:N:171:PRO:HG2	14:N:174:MET:HG3	1.98	0.44
15:O:216:VAL:N	15:O:229:ARG:O	2.49	0.44
17:Q:210:GLU:O	17:Q:214:LEU:HB2	2.17	0.44
18:R:261:ALA:HB1	18:R:264:LEU:HD12	1.99	0.44
19:S:273:VAL:HG13	19:S:304:VAL:HG12	1.99	0.44
21:U:31:PRO:CB	21:U:60:ARG:NH1	2.67	0.44
27:BA:67:LEU:HD12	27:BA:67:LEU:HA	1.86	0.44
44:BM:140:ARG:HG3	44:BM:141:ARG:HH11	1.82	0.44
44:BM:141:ARG:HH21	44:BM:272:LYS:HE2	1.82	0.44
44:BM:221:ARG:HD2	44:BM:228:ASN:OD1	2.17	0.44
44:BM:222:MET:HG3	44:BM:224:PRO:HD3	1.99	0.44
44:BM:288:ALA:HB1	44:BM:306:LEU:HD21	2.00	0.44
65:BL:360:GLN:HB2	65:BL:365:LEU:HD21	2.00	0.44
71:1:270:A:C5	71:1:306:A:N6	2.85	0.44
71:1:845:A:H2	71:1:850:U:O4	2.01	0.44
71:1:876:G:H3'	71:1:877:G:H8	1.82	0.44
1:A:312:LYS:NZ	1:A:368:ALA:HA	2.31	0.44
3:C:204:GLU:OE1	3:C:204:GLU:N	2.51	0.44
7:G:23:PHE:HA	7:G:26:ASN:OD1	2.17	0.44
8:H:35:PRO:HB2	8:H:56:PHE:HB2	1.98	0.44
11:K:16:GLU:N	11:K:16:GLU:OE2	2.50	0.44
15:O:67:ILE:HB	71:1:134:A:C6	2.53	0.44
15:O:113:HIS:O	15:O:117:GLN:HB2	2.18	0.44
15:O:169:GLN:HG2	15:O:170:ASN:OD1	2.18	0.44
15:O:260:GLN:H	15:O:260:GLN:CD	2.19	0.44
17:Q:35:ILE:HD12	61:BD:29:ILE:HD12	1.99	0.44
18:R:50:ILE:HG22	26:Z:153:TYR:CG	2.53	0.44
24:X:320:VAL:HG21	24:X:400:VAL:HG11	2.00	0.44
26:Z:76:ARG:CZ	71:1:71:A:O4'	2.65	0.44
26:Z:76:ARG:NH2	71:1:70:G:O5'	2.51	0.44
27:BA:67:LEU:HG	27:BA:113:MET:HA	1.99	0.44
29:BB:92:ASN:OD1	29:BB:93:THR:HG23	2.18	0.44
34:BI:146:TYR:OH	34:BI:210:SER:O	2.21	0.44
44:BM:169:ILE:HG21	44:BM:175:GLN:HE21	1.82	0.44
44:BM:210:ALA:HB2	44:BM:239:VAL:HG21	2.00	0.44
52:BP:97:ARG:HH21	52:BP:97:ARG:HB2	1.82	0.44
65:BL:155:ILE:HB	65:BL:177:TYR:CE1	2.53	0.44
66:BO:60:LEU:HG	66:BO:133:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:BO:104:GLN:O	66:BO:105:ARG:HD3	2.18	0.44
71:1:124:A:H2'	71:1:125:A:O4'	2.18	0.44
71:1:145:A:H2'	71:1:146:U:H5"	1.98	0.44
71:1:508:G:O2'	71:1:519:U:O4	2.24	0.44
71:1:539:U:C2	71:1:540:U:O2	2.71	0.44
71:1:645:G:N1	71:1:646:U:O2	2.51	0.44
1:A:48:ASP:OD1	1:A:48:ASP:N	2.50	0.44
1:A:70:ILE:HD11	1:A:77:TRP:CZ2	2.52	0.44
1:A:144:TYR:CE2	1:A:150:GLN:HB2	2.53	0.44
3:C:173:SER:HB2	3:C:176:GLU:HB2	1.99	0.44
4:D:121:ALA:O	4:D:125:PHE:N	2.31	0.44
5:E:72:PHE:HB3	5:E:77:LEU:HB2	2.00	0.44
6:F:16:LEU:O	6:F:54:ILE:HA	2.18	0.44
7:G:43:LYS:HD3	7:G:43:LYS:HA	1.85	0.44
7:G:110:HIS:O	7:G:112:VAL:N	2.51	0.44
9:I:40:THR:O	9:I:40:THR:OG1	2.29	0.44
10:J:66:PRO:HG3	66:BO:185:LEU:HD11	1.99	0.44
10:J:92:TYR:HE1	10:J:99:ASN:HB3	1.82	0.44
15:O:231:ILE:HG22	15:O:238:LEU:HA	2.00	0.44
16:P:161:ARG:CD	16:P:181:ARG:HE	2.30	0.44
18:R:208:TRP:HD1	18:R:213:THR:HG23	1.83	0.44
18:R:259:VAL:O	18:R:261:ALA:N	2.51	0.44
20:T:72:TRP:CE2	20:T:82:LYS:HB3	2.52	0.44
21:U:31:PRO:HG2	71:1:951:U:C1'	2.48	0.44
23:W:94:LYS:HD2	23:W:94:LYS:H	1.82	0.44
25:Y:40:TRP:CD1	37:BC:113:LYS:HE3	2.53	0.44
26:Z:76:ARG:NH1	71:1:71:A:C4	2.86	0.44
28:UA:140:UNK:O	28:UA:144:UNK:N	2.51	0.44
50:BE:91:ILE:H	50:BE:91:ILE:HD12	1.82	0.44
66:BO:73:ASN:ND2	66:BO:119:ARG:HD3	2.33	0.44
66:BO:121:LYS:HB2	66:BO:124:ASN:ND2	2.33	0.44
67:BG:1304:MET:HB3	67:BG:1304:MET:HE2	1.88	0.44
71:1:784:A:N1	71:1:787:G:C6	2.86	0.44
71:1:798:A:O2'	71:1:799:A:O4'	2.36	0.44
71:1:960:A:O2'	71:1:961:A:OP1	2.32	0.44
2:B:383:ALA:HB1	18:R:222:TYR:CZ	2.53	0.44
3:C:18:HIS:HB3	3:C:27:PRO:HD2	1.98	0.44
7:G:120:ILE:HG21	13:M:19:GLN:HE21	1.82	0.44
9:I:85:VAL:HG22	9:I:89:ARG:HB2	2.00	0.44
9:I:238:ARG:NH1	15:O:88:ARG:HB2	2.33	0.44
14:N:118:GLU:OE1	14:N:139:PRO:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:112:SER:O	15:O:116:ILE:HG12	2.18	0.44
15:O:156:ILE:HG23	15:O:166:ILE:HG23	2.00	0.44
16:P:94:ILE:HD11	16:P:152:VAL:HG11	1.99	0.44
24:X:192:PRO:HA	24:X:193:PRO:HD3	1.87	0.44
24:X:345:THR:HG23	24:X:403:ALA:O	2.18	0.44
27:BA:130:LEU:O	27:BA:133:TRP:N	2.50	0.44
44:BM:244:LEU:HD11	44:BM:348:ARG:HH11	1.83	0.44
44:BM:246:ARG:NE	44:BM:267:GLY:O	2.50	0.44
50:BE:56:HIS:CE1	50:BE:59:GLU:HB3	2.53	0.44
65:BL:129:LEU:N	65:BL:129:LEU:CD1	2.81	0.44
66:BO:40:LYS:HA	66:BO:40:LYS:HD2	1.40	0.44
71:1:169:U:O4	71:1:170:A:N6	2.51	0.44
71:1:355:U:C2	71:1:356:A:C8	3.06	0.44
71:1:629:A:C8	71:1:631:C:N4	2.86	0.44
71:1:640:A:C2	71:1:799:A:C2	3.06	0.44
71:1:933:G:H2'	71:1:934:G:N7	2.33	0.44
71:1:1033:U:H2'	71:1:1034:C:C6	2.53	0.44
1:A:276:MET:HG3	71:1:865:A:H4'	2.00	0.44
1:A:384:ARG:HD3	66:BO:140:MET:SD	2.57	0.44
7:G:21:VAL:HG23	7:G:21:VAL:O	2.18	0.44
7:G:139:LYS:HB2	14:N:52:LEU:HD11	1.99	0.44
9:I:11:ARG:NH1	9:I:11:ARG:O	2.51	0.44
13:M:210:ASP:O	13:M:225:THR:OG1	2.26	0.44
18:R:35:PRO:HG2	18:R:38:SER:HB2	2.00	0.44
18:R:185:LYS:HE3	18:R:185:LYS:HB3	1.65	0.44
21:U:45:ALA:O	21:U:47:THR:HG22	2.18	0.44
24:X:363:PHE:CD1	24:X:387:PRO:HD3	2.52	0.44
25:Y:267:SER:O	25:Y:267:SER:OG	2.36	0.44
26:Z:104:LYS:NZ	71:1:552:A:OP2	2.39	0.44
44:BM:246:ARG:HG2	44:BM:266:TRP:CE3	2.53	0.44
71:1:320:G:H4'	71:1:321:U:O5'	2.18	0.44
71:1:433:G:O6	71:1:452:A:N6	2.46	0.44
71:1:474:U:HO2'	71:1:475:A:P	2.41	0.44
71:1:1036:U:C4	71:1:1057:A:C5	3.06	0.44
1:A:70:ILE:HA	1:A:83:GLN:NE2	2.33	0.43
2:B:248:LEU:HD12	2:B:248:LEU:HA	1.85	0.43
2:B:410:ALA:HB2	2:B:423:ARG:NH1	2.32	0.43
5:E:162:GLN:HB3	5:E:168:VAL:O	2.19	0.43
6:F:16:LEU:HD21	6:F:26:VAL:HG13	1.98	0.43
7:G:17:VAL:O	7:G:20:THR:HG22	2.18	0.43
7:G:142:TRP:O	7:G:145:ARG:NH2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:257:MET:SD	7:G:262:LEU:HA	2.57	0.43
9:I:44:LEU:HD22	9:I:99:HIS:HB3	2.00	0.43
9:I:145:MET:HE3	9:I:164:GLU:HG3	1.99	0.43
12:L:133:LYS:N	12:L:149:ASN:HD21	2.15	0.43
16:P:141:ASP:OD1	16:P:148:TRP:NE1	2.50	0.43
17:Q:137:ASP:HB2	17:Q:160:LEU:HD21	2.00	0.43
17:Q:215:MET:O	17:Q:218:ARG:HB3	2.18	0.43
19:S:277:LEU:HD11	19:S:307:VAL:HG11	2.00	0.43
25:Y:96:MET:HB3	37:BC:22:HIS:CD2	2.53	0.43
29:BB:35:GLU:O	29:BB:39:SER:OG	2.25	0.43
44:BM:235:LYS:C	44:BM:238:PRO:HD2	2.38	0.43
44:BM:276:HIS:HA	44:BM:279:TYR:CE2	2.53	0.43
71:1:496:U:C5	71:1:497:A:C4	3.06	0.43
71:1:983:U:H3'	71:1:984:A:C5'	2.46	0.43
71:1:1114:A:O2'	71:1:1115:U:H5'	2.19	0.43
3:C:144:ALA:HA	3:C:148:LEU:HB2	1.99	0.43
3:C:177:GLU:HG2	61:BD:58:VAL:N	2.27	0.43
9:I:173:ASN:HB2	9:I:174:HIS:HD2	1.82	0.43
16:P:53:PHE:CB	16:P:60:ARG:HE	2.29	0.43
18:R:143:LEU:HD11	18:R:358:VAL:HG21	2.00	0.43
19:S:266:PRO:HG3	19:S:283:GLU:O	2.17	0.43
21:U:17:ARG:O	21:U:18:LEU:HB3	2.18	0.43
22:V:22:ARG:NH2	71:1:314:A:H4'	2.28	0.43
23:W:89:CYS:SG	23:W:92:HIS:O	2.76	0.43
26:Z:42:ASN:N	26:Z:42:ASN:OD1	2.49	0.43
65:BL:259:LEU:HD21	65:BL:267:PHE:CE1	2.53	0.43
66:BO:36:ILE:HD11	66:BO:38:ARG:NH1	2.32	0.43
71:1:107:U:H5'	71:1:108:U:H5'	2.00	0.43
71:1:109:U:O2'	71:1:110:U:OP2	2.36	0.43
71:1:164:U:OP2	71:1:166:U:N3	2.51	0.43
71:1:567:A:O2'	71:1:568:A:P	2.76	0.43
71:1:826:A:N6	71:1:827:A:N1	2.66	0.43
71:1:913:A:H5'	71:1:914:U:OP2	2.18	0.43
1:A:235:GLN:HG2	1:A:236:GLU:H	1.83	0.43
1:A:235:GLN:HG2	1:A:236:GLU:N	2.33	0.43
5:E:179:ARG:HD3	71:1:432:U:O4'	2.19	0.43
8:H:72:LEU:HB3	8:H:77:ARG:NH2	2.30	0.43
9:I:103:LEU:HD13	9:I:115:LEU:HB2	2.01	0.43
15:O:159:VAL:N	18:R:439:SER:OG	2.41	0.43
15:O:202:HIS:O	15:O:211:CYS:N	2.36	0.43
18:R:203:GLU:HG3	18:R:314:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:261:ALA:O	18:R:264:LEU:HB2	2.19	0.43
19:S:351:HIS:O	19:S:354:SER:N	2.50	0.43
23:W:91:ALA:O	23:W:92:HIS:C	2.56	0.43
24:X:334:THR:HB	24:X:415:THR:HB	2.00	0.43
24:X:484:ARG:HD2	24:X:511:TYR:HE1	1.83	0.43
27:BA:116:VAL:HG13	27:BA:143:VAL:HA	2.01	0.43
37:BC:91:ARG:N	37:BC:91:ARG:HD2	2.33	0.43
71:1:105:A:O3'	71:1:106:A:H4'	2.17	0.43
71:1:163:U:N3	71:1:1013:U:H5'	2.34	0.43
71:1:383:A:H2'	71:1:384:A:O4'	2.18	0.43
71:1:509:U:O2	71:1:513:U:O2'	2.26	0.43
71:1:509:U:C2	71:1:513:U:H1'	2.53	0.43
71:1:510:U:H5	71:1:513:U:H4'	1.84	0.43
71:1:682:A:C6	71:1:683:U:C4	3.06	0.43
71:1:910:U:HO2'	71:1:911:A:P	2.41	0.43
71:1:975:U:C2	71:1:976:A:H2	2.36	0.43
71:1:991:G:N2	71:1:992:G:C4	2.86	0.43
71:1:1045:U:OP2	71:1:1070:C:H4'	2.18	0.43
2:B:15:ARG:NH2	71:1:516:A:OP2	2.43	0.43
2:B:409:GLU:CD	2:B:409:GLU:H	2.22	0.43
3:C:162:TYR:HD1	3:C:167:LEU:HB2	1.83	0.43
17:Q:169:LYS:O	17:Q:172:VAL:HG22	2.19	0.43
17:Q:173:LEU:HD23	17:Q:173:LEU:HA	1.79	0.43
18:R:280:LEU:HD23	18:R:281:GLU:HG3	2.00	0.43
24:X:278:ARG:HG2	24:X:279:HIS:NE2	2.32	0.43
26:Z:43:ILE:O	26:Z:44:LEU:CB	2.64	0.43
44:BM:119:THR:HG23	44:BM:122:LEU:HB2	1.99	0.43
52:BP:158:PRO:HB3	52:BP:160:TRP:CZ2	2.52	0.43
65:BL:213:SER:OG	65:BL:216:GLU:OE2	2.35	0.43
66:BO:47:TRP:HB2	71:1:814:A:C2	2.53	0.43
66:BO:187:ASN:CG	66:BO:188:PHE:H	2.21	0.43
71:1:228:G:N2	71:1:304:G:H2'	2.32	0.43
71:1:574:A:O2'	71:1:575:G:C8	2.69	0.43
71:1:772:U:C5	71:1:773:A:C6	3.06	0.43
71:1:881:G:C8	71:1:987:A:C2	3.06	0.43
71:1:1110:G:H3'	71:1:1111:C:H5'	2.01	0.43
1:A:392:LEU:HD13	10:J:64:TYR:CE2	2.53	0.43
2:B:82:THR:O	2:B:87:LYS:NZ	2.43	0.43
3:C:136:THR:HG21	3:C:172:HIS:CE1	2.54	0.43
4:D:19:SER:OG	4:D:22:LEU:HD12	2.18	0.43
5:E:206:THR:O	5:E:210:TYR:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:264:LEU:HD13	5:E:297:TRP:CE2	2.53	0.43
10:J:67:ARG:CZ	10:J:67:ARG:CB	2.94	0.43
10:J:133:ASP:O	10:J:137:LEU:HD23	2.19	0.43
11:K:66:VAL:O	11:K:70:ALA:N	2.44	0.43
11:K:140:ASP:HB2	11:K:143:VAL:HG22	1.99	0.43
12:L:89:MET:HG3	12:L:113:ALA:HB3	1.99	0.43
13:M:15:ALA:O	13:M:35:GLU:HB2	2.19	0.43
16:P:61:GLN:NE2	16:P:65:ARG:HD3	2.33	0.43
17:Q:108:ILE:HG21	71:1:905:A:N7	2.34	0.43
21:U:25:PHE:O	21:U:25:PHE:CG	2.65	0.43
22:V:25:VAL:HG22	22:V:26:LEU:N	2.29	0.43
23:W:60:HIS:HE1	23:W:94:LYS:HB3	1.83	0.43
29:BB:46:VAL:HG22	29:BB:47:ALA:H	1.83	0.43
29:BB:100:GLU:O	29:BB:104:LYS:HB2	2.18	0.43
37:BC:136:GLU:OE2	37:BC:139:PRO:HA	2.18	0.43
47:BH:74:LEU:HD23	47:BH:106:VAL:HG12	2.01	0.43
52:BP:140:THR:HG23	52:BP:140:THR:O	2.18	0.43
54:BF:53:LEU:HD12	54:BF:57:TYR:CE2	2.53	0.43
71:1:217:A:H62	71:1:323:A:N6	2.08	0.43
71:1:434:U:O4’	71:1:443:G:H1’	2.18	0.43
71:1:699:A:O2’	71:1:700:U:O4’	2.32	0.43
71:1:711:A:H5”	71:1:712:U:C5	2.54	0.43
71:1:876:G:N1	71:1:991:G:N2	2.67	0.43
71:1:1068:A:H2’	71:1:1096:A:N6	2.32	0.43
71:1:1080:A:H8	71:1:1088:G:C2	2.36	0.43
71:1:1122:A:O2’	71:1:1123:U:OP2	2.31	0.43
2:B:152:LYS:HE2	2:B:165:GLY:HA3	2.00	0.43
2:B:246:GLY:HA3	2:B:275:ARG:HG2	2.01	0.43
5:E:138:PRO:HG2	5:E:141:LEU:HD13	2.00	0.43
6:F:157:ASP:OD1	6:F:157:ASP:N	2.52	0.43
8:H:77:ARG:HA	8:H:77:ARG:HD3	1.61	0.43
10:J:5:ARG:NH2	71:1:1109:A:OP2	2.52	0.43
13:M:99:LEU:HD21	13:M:108:GLN:HG2	2.00	0.43
14:N:95:TYR:CZ	14:N:97:GLY:HA3	2.53	0.43
16:P:40:VAL:HG11	16:P:46:LEU:HD21	2.00	0.43
16:P:139:GLU:O	16:P:143:VAL:HG23	2.19	0.43
18:R:19:GLY:O	18:R:23:ASN:ND2	2.52	0.43
18:R:373:ALA:HB1	18:R:379:TYR:CE1	2.54	0.43
22:V:132:ARG:HD3	71:1:103:U:C5	2.54	0.43
29:BB:112:LEU:HB3	29:BB:113:PRO:HD2	2.01	0.43
34:BI:261:VAL:HG23	34:BI:262:GLU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BP:70:PRO:HD2	52:BP:85:PHE:CZ	2.54	0.43
65:BL:84:GLN:HG3	65:BL:291:LYS:HD2	1.99	0.43
65:BL:310:ARG:NH1	71:1:297:U:H3	2.01	0.43
66:BO:65:LYS:HB3	66:BO:78:ARG:HG3	2.00	0.43
67:BG:1341:VAL:HG23	67:BG:1342:CYS:N	2.30	0.43
71:1:46:U:H2'	71:1:47:A:N7	2.33	0.43
71:1:190:A:H61	71:1:207:G:H2'	1.77	0.43
71:1:390:A:H2	71:1:391:A:C4	2.36	0.43
71:1:949:U:N3	71:1:950:A:N7	2.67	0.43
71:1:1079:A:N6	71:1:1080:A:N7	2.66	0.43
1:A:284:ILE:O	1:A:285:TYR:C	2.57	0.43
3:C:185:TYR:O	3:C:188:LEU:N	2.51	0.43
5:E:261:ASP:OD1	5:E:261:ASP:N	2.52	0.43
12:L:145:ASP:OD1	12:L:145:ASP:N	2.51	0.43
14:N:75:GLU:C	14:N:77:ASN:H	2.22	0.43
15:O:178:ILE:HG12	18:R:435:LEU:HD21	2.01	0.43
22:V:122:SER:O	22:V:122:SER:OG	2.27	0.43
24:X:362:ASP:N	24:X:362:ASP:OD1	2.51	0.43
26:Z:105:LEU:O	26:Z:107:PHE:N	2.52	0.43
27:BA:91:HIS:CD2	27:BA:93:HIS:H	2.37	0.43
34:BI:83:PHE:HB2	34:BI:95:ARG:HG3	2.01	0.43
44:BM:210:ALA:HB3	44:BM:236:LEU:HA	2.00	0.43
44:BM:364:GLN:O	44:BM:367:VAL:HG12	2.18	0.43
66:BO:51:THR:HG22	66:BO:144:GLN:NE2	2.34	0.43
66:BO:87:ARG:HG3	66:BO:133:ARG:NH1	2.33	0.43
71:1:170:A:O2'	71:1:172:A:OP2	2.31	0.43
71:1:559:U:HO2'	71:1:560:U:P	2.39	0.43
71:1:855:A:O5'	71:1:855:A:H8	2.02	0.43
71:1:886:A:C2	71:1:980:A:C4	3.07	0.43
71:1:934:G:HO2'	71:1:935:G:P	2.42	0.43
1:A:312:LYS:NZ	1:A:367:LEU:O	2.29	0.43
7:G:298:LEU:HD23	7:G:298:LEU:HA	1.86	0.43
8:H:56:PHE:CE1	52:BP:183:ILE:HD13	2.52	0.43
9:I:72:ARG:NH1	71:1:544:U:H2'	2.33	0.43
9:I:228:ARG:NH1	9:I:232:LEU:HD21	2.34	0.43
10:J:48:HIS:NE2	10:J:52:GLN:HG2	2.33	0.43
10:J:79:HIS:HB3	10:J:87:GLY:O	2.19	0.43
13:M:15:ALA:HA	13:M:16:PRO:HD3	1.91	0.43
13:M:178:ARG:HA	13:M:178:ARG:HD3	1.79	0.43
16:P:30:LYS:NZ	16:P:48:GLU:OE2	2.33	0.43
16:P:161:ARG:NH1	16:P:181:ARG:HH21	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:82:VAL:O	17:Q:82:VAL:HG23	2.18	0.43
19:S:292:PRO:HB2	19:S:294:ILE:HG23	2.01	0.43
24:X:494:LEU:N	24:X:494:LEU:CD1	2.81	0.43
24:X:499:ARG:O	24:X:502:MET:HG2	2.19	0.43
37:BC:101:SER:OG	37:BC:104:ARG:NH2	2.52	0.43
44:BM:101:LYS:HG2	44:BM:108:LEU:HD13	1.99	0.43
44:BM:251:ARG:HE	44:BM:253:CYS:HB2	1.84	0.43
65:BL:119:ARG:HH11	65:BL:132:HIS:CA	2.32	0.43
65:BL:200:ALA:HB2	65:BL:205:LEU:HD23	2.01	0.43
66:BO:92:ARG:O	66:BO:95:PRO:HD2	2.19	0.43
66:BO:176:HIS:HD2	66:BO:178:TYR:N	2.16	0.43
68:UB:5:UNK:C	68:UB:7:UNK:H	2.32	0.43
68:UB:38:UNK:O	68:UB:39:UNK:C	2.66	0.43
71:1:71:A:H61	71:1:75:A:H61	1.67	0.43
71:1:420:A:O2'	71:1:421:U:H5"	2.19	0.43
5:E:75:LEU:HB3	5:E:110:LYS:NZ	2.34	0.43
8:H:95:GLN:HA	8:H:109:ILE:CG1	2.46	0.43
9:I:175:LYS:N	9:I:201:ARG:HH12	1.97	0.43
13:M:144:LYS:HB3	13:M:144:LYS:HE2	1.76	0.43
14:N:162:GLU:HG2	14:N:228:PRO:HB2	2.01	0.43
14:N:170:ILE:HG21	14:N:179:LEU:HD13	2.01	0.43
15:O:29:ARG:CG	15:O:33:ARG:HD3	2.48	0.43
17:Q:108:ILE:CG1	71:1:905:A:H62	2.31	0.43
18:R:54:LEU:HD22	18:R:87:VAL:HG23	2.01	0.43
21:U:19:LYS:O	21:U:19:LYS:HG2	2.19	0.43
24:X:234:ALA:H	24:X:237:ALA:HA	1.84	0.43
24:X:343:LYS:HD3	24:X:409:CYS:SG	2.59	0.43
25:Y:93:ILE:HD11	37:BC:41:VAL:HG21	2.01	0.43
27:BA:74:GLU:HG2	27:BA:75:PRO:HD3	2.00	0.43
44:BM:46:ARG:HH21	44:BM:50:LYS:HZ3	1.67	0.43
47:BH:152:LEU:HD22	47:BH:156:PHE:CD2	2.54	0.43
52:BP:-4:THR:HB	71:1:487:U:OP2	2.19	0.43
65:BL:133:TYR:CD2	65:BL:303:LYS:HG2	2.54	0.43
65:BL:141:TRP:O	65:BL:141:TRP:HD1	1.98	0.43
65:BL:284:ASN:HB2	71:1:671:U:C2	2.54	0.43
65:BL:330:LEU:HD12	65:BL:330:LEU:O	2.19	0.43
66:BO:68:CYS:SG	66:BO:76:HIS:HB3	2.58	0.43
71:1:503:U:O2'	71:1:504:U:OP2	2.31	0.43
71:1:556:A:OP2	71:1:557:A:H2'	2.19	0.43
71:1:581:U:H5'	71:1:582:U:C5	2.54	0.43
71:1:763:G:H4'	71:1:764:U:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:974:U:O2	71:1:974:U:H2'	2.18	0.43
6:F:112:VAL:O	6:F:118:ARG:HD3	2.19	0.43
9:I:152:ARG:NH1	9:I:157:ASN:HB3	2.34	0.43
10:J:64:TYR:CD2	10:J:64:TYR:C	2.92	0.43
13:M:76:ASN:O	13:M:78:PRO:HD3	2.19	0.43
15:O:21:TYR:OH	15:O:28:ALA:HA	2.19	0.43
15:O:112:SER:O	15:O:115:LYS:HB3	2.19	0.43
17:Q:141:LEU:HD23	17:Q:141:LEU:HA	1.74	0.43
18:R:246:ASN:HD22	18:R:255:ALA:HB1	1.83	0.43
20:T:29:PRO:HA	71:1:1101:C:H1'	2.00	0.43
24:X:93:GLN:HG3	24:X:94:LEU:N	2.34	0.43
26:Z:110:GLY:N	71:1:572:A:OP1	2.52	0.43
34:BI:182:ASP:HB2	34:BI:206:HIS:HA	2.00	0.43
61:BD:58:VAL:HG13	61:BD:71:SER:HB2	1.99	0.43
61:BD:63:CYS:SG	61:BD:64:HIS:N	2.92	0.43
65:BL:157:LYS:HA	65:BL:177:TYR:HA	2.01	0.43
65:BL:259:LEU:HD21	65:BL:267:PHE:HE1	1.83	0.43
66:BO:80:ILE:HB	66:BO:102:SER:HB2	2.01	0.43
71:1:861:A:C2	71:1:862:A:C5	3.07	0.43
71:1:863:A:N6	71:1:864:A:C6	2.86	0.43
1:A:261:TYR:CB	1:A:264:LEU:HB2	2.49	0.42
2:B:133:GLN:NE2	13:M:10:ILE:HD13	2.34	0.42
2:B:140:ASP:OD1	2:B:141:TYR:N	2.52	0.42
2:B:364:SER:O	2:B:364:SER:OG	2.34	0.42
3:C:122:TRP:HD1	3:C:129:TRP:NE1	2.17	0.42
7:G:115:MET:HE3	7:G:115:MET:HB3	1.97	0.42
9:I:116:ALA:HA	9:I:125:VAL:HG11	2.01	0.42
9:I:226:ARG:O	9:I:243:PRO:HB3	2.18	0.42
11:K:45:THR:HG21	71:1:153:U:O2	2.18	0.42
12:L:86:GLN:OE1	12:L:114:THR:HB	2.18	0.42
13:M:159:ARG:HE	13:M:243:LEU:HD13	1.84	0.42
18:R:116:ARG:HH11	18:R:121:ILE:HD11	1.83	0.42
21:U:17:ARG:HB2	21:U:19:LYS:HE2	2.01	0.42
22:V:37:MET:HG3	22:V:39:VAL:HG23	2.01	0.42
26:Z:76:ARG:NE	71:1:71:A:O4'	2.51	0.42
34:BI:249:THR:HG22	34:BI:253:GLU:O	2.19	0.42
44:BM:17:ARG:NH2	44:BM:19:PHE:HB3	2.32	0.42
44:BM:98:LYS:HA	44:BM:123:GLN:NE2	2.34	0.42
44:BM:188:LYS:C	44:BM:191:GLU:HG2	2.39	0.42
47:BH:68:GLY:HA2	47:BH:214:HIS:CE1	2.52	0.42
52:BP:-12:LEU:O	52:BP:-11:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:BD:63:CYS:SG	61:BD:65:ARG:N	2.90	0.42
68:UB:63:UNK:O	68:UB:67:UNK:N	2.53	0.42
71:1:235:G:N2	71:1:236:A:C5	2.86	0.42
71:1:318:U:N3	71:1:319:A:N7	2.67	0.42
71:1:353:A:H61	71:1:373:A:N6	2.17	0.42
71:1:662:G:N2	71:1:675:A:C2	2.87	0.42
71:1:700:U:C3'	71:1:701:U:H5'	2.49	0.42
71:1:763:G:H2'	71:1:764:U:H3'	2.01	0.42
71:1:803:U:H2'	71:1:804:U:O4'	2.19	0.42
71:1:910:U:H2'	71:1:911:A:O4'	2.19	0.42
71:1:1029:U:H3	71:1:1057:A:N6	2.17	0.42
71:1:1039:A:H61	71:1:1051:A:H61	1.67	0.42
4:D:27:ARG:NE	4:D:29:TYR:HH	2.17	0.42
5:E:249:PRO:HG3	5:E:309:VAL:HG22	2.01	0.42
8:H:13:ARG:CZ	8:H:13:ARG:HA	2.49	0.42
9:I:73:MET:CE	9:I:89:ARG:HH11	2.33	0.42
10:J:34:ALA:O	10:J:38:ILE:HG23	2.18	0.42
10:J:142:ARG:HD2	71:1:806:A:OP2	2.18	0.42
11:K:24:LEU:HD11	11:K:39:ILE:HB	2.00	0.42
11:K:44:ARG:HD2	12:L:97:SER:O	2.19	0.42
13:M:149:GLU:HG2	13:M:170:ARG:HD3	2.01	0.42
14:N:47:ARG:NH1	71:1:91:U:OP1	2.52	0.42
17:Q:219:VAL:O	17:Q:222:GLN:HB3	2.18	0.42
18:R:211:SER:C	18:R:213:THR:H	2.21	0.42
19:S:260:VAL:HG12	19:S:282:LEU:HD11	2.01	0.42
21:U:31:PRO:HG2	71:1:951:U:C2	2.54	0.42
22:V:45:LYS:HE3	71:1:194:U:OP2	2.19	0.42
24:X:67:GLN:HG3	24:X:69:PRO:HD2	2.01	0.42
24:X:198:MET:HE1	24:X:227:PHE:HE2	1.84	0.42
24:X:481:LEU:HD12	24:X:482:PRO:CD	2.49	0.42
44:BM:15:ASN:OD1	44:BM:16:TYR:N	2.52	0.42
44:BM:178:ALA:O	44:BM:182:ARG:HB3	2.20	0.42
52:BP:96:PRO:C	52:BP:98:PRO:HD2	2.37	0.42
65:BL:257:LEU:HD12	65:BL:267:PHE:CD1	2.53	0.42
65:BL:337:ARG:HB3	71:1:707:U:O2'	2.19	0.42
66:BO:44:ARG:HD3	66:BO:44:ARG:HA	1.78	0.42
71:1:478:A:H4'	71:1:480:A:N6	2.34	0.42
71:1:617:G:H3'	71:1:617:G:N3	2.34	0.42
71:1:801:A:H2'	71:1:802:U:O4'	2.19	0.42
71:1:864:A:N7	71:1:865:A:C6	2.87	0.42
1:A:128:SER:HB3	1:A:353:PHE:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:PRO:HG3	71:1:1105:G:O5'	2.19	0.42
2:B:425:ILE:HD12	2:B:430:THR:HG21	2.00	0.42
4:D:67:ILE:HD13	4:D:72:VAL:HG13	2.00	0.42
5:E:101:ILE:HG13	5:E:120:PRO:HD3	2.01	0.42
8:H:68:ARG:HG3	8:H:82:LEU:HD23	2.00	0.42
13:M:254:LEU:C	13:M:256:THR:H	2.22	0.42
15:O:114:GLN:HA	15:O:117:GLN:CB	2.48	0.42
15:O:280:ARG:NE	18:R:102:ASP:OD1	2.45	0.42
17:Q:207:ASP:N	17:Q:210:GLU:OE2	2.52	0.42
19:S:295:PRO:CG	19:S:296:PRO:HD3	2.49	0.42
24:X:66:PHE:HB3	24:X:71:GLU:OE1	2.19	0.42
25:Y:147:VAL:O	25:Y:151:ARG:HG2	2.19	0.42
34:BI:138:ASP:O	34:BI:141:LEU:HB3	2.18	0.42
34:BI:141:LEU:HG	34:BI:142:PRO:HD2	2.02	0.42
65:BL:205:LEU:N	65:BL:206:PRO:HD3	2.34	0.42
66:BO:87:ARG:HH11	66:BO:89:ALA:CB	2.31	0.42
66:BO:88:PHE:N	66:BO:88:PHE:CD1	2.87	0.42
66:BO:95:PRO:HG2	66:BO:97:VAL:HG13	2.01	0.42
71:1:111:A:H4'	71:1:112:U:O5'	2.19	0.42
71:1:144:U:H4'	71:1:836:U:H5'	2.01	0.42
71:1:288:C:H2'	71:1:288:C:OP2	2.20	0.42
71:1:520:A:O2'	71:1:521:U:OP2	2.31	0.42
71:1:596:U:H6	71:1:596:U:H2'	1.69	0.42
71:1:936:G:N1	71:1:937:C:C4	2.87	0.42
71:1:1019:C:O5'	71:1:1019:C:H6	2.01	0.42
2:B:93:PRO:HA	2:B:104:THR:HA	2.00	0.42
2:B:150:ALA:HB3	14:N:85:ARG:HH22	1.83	0.42
4:D:33:ARG:NE	4:D:41:CYS:SG	2.91	0.42
5:E:179:ARG:NH1	71:1:432:U:C4	2.87	0.42
6:F:34:MET:O	6:F:49:GLY:HA3	2.20	0.42
7:G:83:ASP:O	7:G:90:ILE:HD11	2.19	0.42
12:L:44:ARG:HA	12:L:114:THR:HG22	2.00	0.42
12:L:132:ASP:OD1	12:L:132:ASP:N	2.46	0.42
15:O:32:THR:OG1	15:O:33:ARG:N	2.52	0.42
15:O:184:ARG:HG2	15:O:185:PRO:HD2	2.00	0.42
16:P:104:GLU:OE1	16:P:104:GLU:HA	2.19	0.42
16:P:151:ARG:HH21	16:P:185:GLU:HG3	1.82	0.42
17:Q:180:LEU:HD23	17:Q:180:LEU:HA	1.88	0.42
18:R:42:LYS:O	18:R:101:ARG:NH2	2.41	0.42
22:V:38:GLN:HA	22:V:41:GLN:HB2	2.00	0.42
24:X:349:PRO:HD3	24:X:398:ARG:HE	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:UA:10:UNK:O	28:UA:14:UNK:N	2.52	0.42
34:BI:167:SER:OG	34:BI:171:THR:O	2.30	0.42
37:BC:77:HIS:CE1	37:BC:79:ALA:HB2	2.53	0.42
44:BM:103:ALA:O	44:BM:107:LEU:HG	2.18	0.42
44:BM:251:ARG:HD2	44:BM:263:ARG:NH2	2.34	0.42
44:BM:285:LEU:HA	44:BM:288:ALA:HB3	2.01	0.42
71:1:314:A:OP2	71:1:314:A:H3'	2.19	0.42
71:1:1031:C:C4	71:1:1035:G:C2	3.07	0.42
1:A:42:MET:HB2	29:BB:75:VAL:HG21	2.02	0.42
1:A:346:GLU:HG2	1:A:347:HIS:H	1.84	0.42
1:A:357:ILE:CD1	29:BB:95:PRO:HG2	2.49	0.42
1:A:384:ARG:HH21	71:1:1149:A:H5"	1.84	0.42
2:B:28:VAL:O	2:B:28:VAL:HG13	2.18	0.42
2:B:170:HIS:HB3	2:B:177:HIS:HA	2.01	0.42
7:G:366:MET:CG	17:Q:28:ARG:HH12	2.30	0.42
8:H:31:LYS:HE3	71:1:388:U:OP2	2.19	0.42
9:I:44:LEU:H	9:I:99:HIS:CD2	2.36	0.42
9:I:187:PHE:HZ	9:I:249:LEU:HB3	1.85	0.42
9:I:244:SER:CB	54:BF:70:ARG:HH22	2.33	0.42
12:L:145:ASP:O	12:L:176:LEU:HD23	2.20	0.42
15:O:22:THR:HG22	15:O:22:THR:O	2.18	0.42
15:O:110:LEU:HD12	15:O:111:GLU:H	1.85	0.42
18:R:145:LEU:O	18:R:330:TRP:N	2.53	0.42
21:U:23:VAL:O	21:U:23:VAL:HG12	2.19	0.42
22:V:38:GLN:O	22:V:42:MET:HG2	2.19	0.42
24:X:294:LEU:HD23	24:X:317:GLY:HA3	2.01	0.42
27:BA:45:GLN:O	27:BA:46:THR:HB	2.20	0.42
29:BB:27:LEU:O	29:BB:30:TYR:HB3	2.20	0.42
37:BC:127:ALA:O	37:BC:131:GLY:N	2.51	0.42
44:BM:162:VAL:HB	44:BM:165:ASP:HB2	2.00	0.42
52:BP:69:ILE:HG23	52:BP:85:PHE:CD1	2.55	0.42
66:BO:36:ILE:HG22	71:1:1128:U:H3	1.85	0.42
71:1:438:G:H2'	71:1:439:A:O4'	2.19	0.42
71:1:538:A:C6	71:1:539:U:C2	3.08	0.42
71:1:551:A:H2'	71:1:552:A:O4'	2.19	0.42
71:1:617:G:C2'	71:1:618:U:H5'	2.50	0.42
71:1:650:U:O2	71:1:650:U:H2'	2.19	0.42
1:A:158:PHE:CE2	1:A:316:ILE:HG21	2.54	0.42
2:B:23:GLU:OE1	2:B:27:GLN:NE2	2.53	0.42
2:B:207:LYS:HA	2:B:207:LYS:HD3	1.66	0.42
2:B:356:LEU:HB3	2:B:361:PHE:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:ARG:HB3	3:C:32:VAL:HG11	2.01	0.42
3:C:77:ARG:CZ	3:C:83:LEU:HD23	2.50	0.42
3:C:79:GLY:O	3:C:95:LYS:NZ	2.52	0.42
3:C:102:ILE:HD12	3:C:102:ILE:H	1.84	0.42
4:D:21:ARG:O	4:D:49:THR:OG1	2.30	0.42
5:E:216:LYS:HG3	5:E:217:HIS:N	2.35	0.42
8:H:6:LEU:HG	8:H:7:ARG:N	2.35	0.42
12:L:22:PHE:HA	12:L:34:VAL:O	2.19	0.42
14:N:154:VAL:HG22	14:N:167:ILE:O	2.19	0.42
15:O:216:VAL:O	15:O:229:ARG:N	2.44	0.42
21:U:67:LYS:NZ	21:U:84:LYS:HD2	2.35	0.42
25:Y:230:ARG:HA	25:Y:233:LEU:HB3	2.02	0.42
25:Y:277:GLU:OE1	25:Y:277:GLU:N	2.52	0.42
26:Z:19:TYR:HB2	71:1:907:G:C2	2.53	0.42
27:BA:69:ILE:HD12	27:BA:95:ILE:HD11	2.01	0.42
47:BH:20:TYR:HD2	47:BH:161:GLN:NE2	2.17	0.42
52:BP:-23:PRO:HG2	52:BP:-21:TYR:CZ	2.55	0.42
66:BO:91:CYS:C	66:BO:93:VAL:N	2.73	0.42
66:BO:130:LEU:O	66:BO:173:HIS:CE1	2.70	0.42
66:BO:165:ARG:NH2	66:BO:167:MET:SD	2.93	0.42
67:BG:1308:MET:HB2	67:BG:1315:THR:HG21	2.02	0.42
69:UC:70:UNK:O	69:UC:74:UNK:N	2.52	0.42
71:1:127:A:C2'	71:1:128:U:H5'	2.49	0.42
71:1:128:U:O2'	71:1:129:U:O4'	2.37	0.42
71:1:698:G:H2'	71:1:699:A:H5"	2.02	0.42
71:1:1043:A:O5'	71:1:1043:A:H8	2.03	0.42
1:A:393:VAL:CG2	1:A:397:ASP:HB3	2.49	0.42
4:D:123:ARG:O	4:D:127:LEU:N	2.53	0.42
5:E:38:ILE:HG22	5:E:89:ARG:HG2	2.01	0.42
5:E:219:LYS:HB2	5:E:219:LYS:HE3	1.81	0.42
6:F:101:TRP:HE3	29:BB:12:PHE:CE2	2.37	0.42
7:G:68:THR:O	7:G:72:GLU:HG2	2.19	0.42
7:G:145:ARG:HG2	71:1:346:A:H5"	2.02	0.42
7:G:197:LEU:O	7:G:197:LEU:HD23	2.19	0.42
8:H:93:VAL:C	8:H:95:GLN:H	2.17	0.42
10:J:73:GLY:HA2	10:J:93:ALA:HA	2.01	0.42
11:K:103:GLU:HG2	12:L:22:PHE:CE1	2.54	0.42
13:M:258:LYS:HD2	13:M:259:ARG:H	1.83	0.42
15:O:276:LEU:HB3	18:R:105:ALA:HB1	2.01	0.42
16:P:64:TYR:O	16:P:79:LEU:HD11	2.20	0.42
18:R:135:HIS:CE1	18:R:372:TYR:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:182:THR:HG23	24:X:189:ILE:HG22	2.02	0.42
27:BA:57:LEU:O	27:BA:61:SER:N	2.50	0.42
27:BA:122:ARG:NE	52:BP:88:ASP:OD1	2.48	0.42
44:BM:141:ARG:HH12	44:BM:268:HIS:HB2	1.84	0.42
65:BL:168:LYS:O	65:BL:170:THR:N	2.53	0.42
71:1:106:A:O2'	71:1:107:U:OP2	2.32	0.42
71:1:826:A:H62	71:1:827:A:N6	2.17	0.42
71:1:860:U:H2'	71:1:861:A:H8	1.85	0.42
71:1:865:A:C5	71:1:1100:U:C4	3.07	0.42
71:1:1000:A:N6	71:1:1009:A:O2'	2.50	0.42
71:1:1067:C:O2'	71:1:1068:A:OP1	2.34	0.42
1:A:393:VAL:HG21	1:A:397:ASP:HB3	2.02	0.42
2:B:191:MET:HG2	2:B:196:TRP:CE3	2.54	0.42
2:B:331:GLY:O	2:B:335:GLN:HG3	2.20	0.42
5:E:206:THR:HG22	5:E:208:LYS:N	2.28	0.42
6:F:22:GLN:O	6:F:26:VAL:HG23	2.20	0.42
6:F:23:LEU:HB3	6:F:24:PRO:HD3	2.01	0.42
6:F:34:MET:SD	6:F:125:ALA:HB2	2.60	0.42
6:F:102:TYR:O	6:F:106:GLU:HG2	2.20	0.42
8:H:98:PRO:HG2	8:H:99:GLU:OE1	2.20	0.42
11:K:48:ARG:O	11:K:52:GLU:HG2	2.19	0.42
11:K:131:GLU:H	11:K:131:GLU:HG3	1.69	0.42
13:M:54:MET:HE2	13:M:54:MET:HB2	1.70	0.42
14:N:78:ARG:HA	14:N:78:ARG:HD2	1.65	0.42
15:O:177:VAL:HG23	15:O:177:VAL:O	2.20	0.42
16:P:53:PHE:N	16:P:60:ARG:HG2	2.34	0.42
16:P:131:ALA:HA	16:P:140:LEU:HD22	2.01	0.42
17:Q:150:SER:OG	17:Q:151:THR:N	2.52	0.42
18:R:118:ALA:O	18:R:371:PRO:HG3	2.20	0.42
21:U:37:ASN:CG	21:U:60:ARG:HG2	2.39	0.42
24:X:303:VAL:HA	24:X:307:VAL:HB	2.01	0.42
25:Y:84:LYS:HA	25:Y:87:GLU:HG2	2.01	0.42
27:BA:20:GLY:HA2	52:BP:-10:ARG:HH11	1.83	0.42
29:BB:88:ARG:HG3	29:BB:89:GLU:N	2.35	0.42
34:BI:126:SER:O	34:BI:131:ILE:HG22	2.19	0.42
44:BM:141:ARG:HH22	44:BM:268:HIS:N	2.17	0.42
65:BL:266:LEU:HG	65:BL:351:LEU:HD13	2.02	0.42
66:BO:82:LYS:HD3	66:BO:82:LYS:HA	1.80	0.42
66:BO:86:GLU:O	66:BO:87:ARG:HB2	2.19	0.42
71:1:75:A:H8	71:1:75:A:O5'	2.02	0.42
71:1:130:U:N3	71:1:131:U:C4	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:391:A:C8	71:1:393:A:N6	2.87	0.42
71:1:567:A:C8	71:1:568:A:C8	3.08	0.42
71:1:646:U:H2'	71:1:647:U:C6	2.54	0.42
1:A:208:VAL:CG2	10:J:12:PHE:HA	2.50	0.42
4:D:108:MET:O	4:D:111:ARG:HG3	2.20	0.42
5:E:186:ARG:NH2	71:1:458:A:H61	2.17	0.42
8:H:139:GLU:HB3	52:BP:171:PHE:HB2	2.01	0.42
9:I:187:PHE:HB3	9:I:216:PHE:HD2	1.84	0.42
14:N:184:LYS:HE3	14:N:184:LYS:HB2	1.90	0.42
16:P:55:GLN:CB	71:1:949:U:H1'	2.50	0.42
17:Q:106:THR:HG21	71:1:905:A:C6	2.55	0.42
18:R:150:ASP:OD1	18:R:151:GLU:N	2.53	0.42
18:R:177:LEU:HA	18:R:177:LEU:HD23	1.77	0.42
18:R:218:SER:C	18:R:263:ARG:HH22	2.22	0.42
24:X:76:SER:OG	24:X:77:ASP:N	2.53	0.42
29:BB:100:GLU:HA	29:BB:103:TRP:NE1	2.35	0.42
44:BM:101:LYS:HE3	44:BM:126:LEU:HB2	2.02	0.42
44:BM:174:MET:SD	44:BM:216:GLN:HG2	2.60	0.42
65:BL:123:ASN:CG	65:BL:124:PRO:HD2	2.41	0.42
71:1:145:A:C2'	71:1:146:U:H5"	2.49	0.42
71:1:438:G:N2	71:1:447:A:C4	2.88	0.42
71:1:754:A:H3'	71:1:755:G:H5"	2.01	0.42
71:1:933:G:C2	71:1:950:A:N6	2.87	0.42
71:1:1132:U:C4	71:1:1133:U:C2	3.07	0.42
1:A:251:VAL:HG23	1:A:290:MET:O	2.20	0.42
2:B:66:GLU:CD	2:B:72:HIS:HB2	2.41	0.42
2:B:374:LEU:HD12	2:B:374:LEU:HA	1.89	0.42
6:F:23:LEU:HD12	6:F:23:LEU:HA	1.79	0.42
6:F:135:HIS:O	6:F:140:PRO:HD3	2.19	0.42
7:G:16:PRO:HG2	7:G:19:GLN:CG	2.50	0.42
7:G:196:THR:OG1	7:G:265:GLU:OE2	2.37	0.42
9:I:43:PRO:N	9:I:45:MET:HE3	2.35	0.42
13:M:53:HIS:CD2	13:M:58:PRO:HB3	2.54	0.42
18:R:398:ASN:HB3	71:1:62:U:O4	2.19	0.42
18:R:415:ALA:O	18:R:419:GLN:HG3	2.20	0.42
25:Y:238:HIS:HA	25:Y:244:ARG:HH21	1.85	0.42
26:Z:12:PHE:O	26:Z:33:ASP:HB2	2.20	0.42
26:Z:68:ARG:HB2	26:Z:79:LEU:HD13	2.02	0.42
27:BA:96:LEU:HD23	27:BA:129:ALA:HB2	2.01	0.42
37:BC:51:ARG:HB3	37:BC:67:ASN:ND2	2.35	0.42
44:BM:155:TYR:O	44:BM:158:MET:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BM:233:VAL:HG22	44:BM:332:ASP:OD2	2.20	0.42
44:BM:366:VAL:HG13	44:BM:370:GLU:HB2	2.01	0.42
47:BH:85:ILE:HG12	47:BH:181:GLY:HA2	2.01	0.42
52:BP:10:TYR:HD1	52:BP:10:TYR:H	1.68	0.42
61:BD:66:CYS:O	61:BD:68:ARG:N	2.53	0.42
65:BL:265:ARG:NH1	71:1:666:A:OP2	2.53	0.42
66:BO:58:VAL:HB	66:BO:135:GLN:HE22	1.85	0.42
66:BO:74:CYS:O	66:BO:76:HIS:ND1	2.53	0.42
71:1:39:U:C1'	71:1:40:C:OP1	2.67	0.42
71:1:231:C:N3	71:1:305:U:H5'	2.35	0.42
71:1:238:U:H6	71:1:238:U:H2'	1.71	0.42
71:1:269:A:N3	71:1:271:U:O2'	2.50	0.42
71:1:424:A:N6	71:1:476:A:OP2	2.53	0.42
71:1:594:U:HO2'	71:1:595:A:C5'	2.33	0.42
71:1:896:A:C4	71:1:915:G:O6	2.72	0.42
71:1:954:A:N1	71:1:970:A:H3'	2.35	0.42
1:A:325:ASP:HB3	9:I:26:GLY:HA3	2.01	0.41
5:E:149:LEU:O	5:E:192:ILE:HG12	2.21	0.41
6:F:113:ARG:HD2	71:1:151:G:OP1	2.20	0.41
7:G:99:GLN:OE1	71:1:183:U:N3	2.52	0.41
7:G:213:TRP:CE2	22:V:140:PRO:HD3	2.55	0.41
7:G:349:GLN:HB3	7:G:350:PRO:HD2	2.02	0.41
9:I:80:LYS:O	9:I:82:TYR:N	2.53	0.41
9:I:145:MET:O	9:I:163:VAL:HA	2.20	0.41
13:M:86:VAL:HA	13:M:90:GLN:O	2.20	0.41
17:Q:67:PRO:HD2	17:Q:73:MET:HE1	2.02	0.41
18:R:57:GLU:O	18:R:61:LEU:N	2.49	0.41
24:X:484:ARG:HD2	24:X:511:TYR:CE1	2.55	0.41
26:Z:106:TYR:OH	26:Z:118:HIS:NE2	2.25	0.41
27:BA:150:ILE:H	27:BA:150:ILE:HG13	1.61	0.41
52:BP:10:TYR:CG	52:BP:11:GLY:N	2.88	0.41
66:BO:172:ARG:CZ	66:BO:172:ARG:CB	2.98	0.41
67:BG:1319:SER:HB2	67:BG:1322:THR:H	1.84	0.41
71:1:355:U:N3	71:1:356:A:N7	2.67	0.41
71:1:792:C:H2'	71:1:793:C:O4'	2.20	0.41
71:1:870:A:H2'	71:1:871:A:C5	2.54	0.41
71:1:875:G:N2	71:1:992:G:O6	2.25	0.41
71:1:1008:A:H3'	71:1:1009:A:O4'	2.19	0.41
1:A:308:ARG:HD3	1:A:373:GLN:HE21	1.85	0.41
7:G:145:ARG:CG	71:1:346:A:H5"	2.50	0.41
8:H:102:MET:O	8:H:102:MET:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:75:GLU:HG3	52:BP:-43:GLU:HA	2.02	0.41
13:M:121:GLU:O	13:M:125:ALA:N	2.52	0.41
13:M:138:ALA:HA	13:M:228:SER:OG	2.20	0.41
15:O:117:GLN:HG2	15:O:121:ARG:HG2	2.02	0.41
16:P:33:HIS:CE1	16:P:45:LYS:HE2	2.56	0.41
17:Q:201:LEU:HD23	17:Q:201:LEU:HA	1.77	0.41
18:R:192:TRP:HE3	18:R:320:PRO:HG2	1.85	0.41
22:V:128:ARG:HA	22:V:128:ARG:HD3	1.77	0.41
23:W:92:HIS:HB3	23:W:95:GLU:HB3	2.01	0.41
26:Z:43:ILE:O	26:Z:43:ILE:HG23	2.18	0.41
29:BB:68:VAL:O	29:BB:68:VAL:HG23	2.20	0.41
44:BM:139:PRO:O	44:BM:142:ARG:N	2.53	0.41
65:BL:123:ASN:OD1	65:BL:124:PRO:HD2	2.19	0.41
65:BL:331:ASP:OD1	65:BL:332:TRP:N	2.46	0.41
66:BO:153:ILE:HG13	66:BO:153:ILE:O	2.20	0.41
71:1:393:A:H4'	71:1:1012:A:C6	2.55	0.41
71:1:557:A:N6	71:1:573:A:N7	2.69	0.41
71:1:753:U:C2	71:1:754:A:C2	3.07	0.41
71:1:952:U:H5"	71:1:953:U:H5'	2.02	0.41
1:A:217:ASP:OD1	1:A:217:ASP:N	2.51	0.41
4:D:109:LEU:HD23	4:D:109:LEU:HA	1.94	0.41
7:G:251:SER:OG	7:G:252:PHE:N	2.53	0.41
10:J:121:SER:OG	10:J:124:HIS:N	2.33	0.41
13:M:36:LEU:HD12	13:M:36:LEU:HA	1.69	0.41
14:N:115:LYS:HZ1	18:R:397:PRO:HD2	1.85	0.41
15:O:192:GLU:OE1	15:O:192:GLU:N	2.53	0.41
16:P:55:GLN:CG	71:1:949:U:H1'	2.51	0.41
16:P:159:THR:OG1	16:P:160:GLU:N	2.53	0.41
18:R:241:SER:HB2	18:R:244:GLU:HB2	2.02	0.41
19:S:367:ARG:HG3	47:BH:137:GLN:NE2	2.35	0.41
22:V:129:SER:O	22:V:133:LYS:HB2	2.21	0.41
24:X:233:ALA:HB3	24:X:237:ALA:HA	2.01	0.41
27:BA:68:VAL:HG12	27:BA:114:PHE:HD2	1.85	0.41
29:BB:128:ASP:O	29:BB:129:THR:HB	2.19	0.41
44:BM:176:ALA:HA	44:BM:179:TYR:CD2	2.55	0.41
44:BM:192:LEU:HD21	44:BM:252:VAL:HG13	2.02	0.41
47:BH:98:LYS:H	47:BH:98:LYS:HD2	1.84	0.41
52:BP:-28:ALA:HB3	52:BP:-25:ALA:HB3	2.02	0.41
65:BL:138:VAL:HG13	65:BL:144:ARG:NE	2.35	0.41
65:BL:327:LEU:O	65:BL:329:PRO:HD3	2.20	0.41
66:BO:87:ARG:NH1	66:BO:89:ALA:HB3	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:181:A:N6	71:1:211:U:OP1	2.54	0.41
71:1:382:A:H3'	71:1:383:A:C8	2.55	0.41
71:1:442:U:O2'	71:1:443:G:OP2	2.38	0.41
71:1:539:U:N3	71:1:540:U:O2	2.53	0.41
71:1:631:C:H4'	71:1:632:A:OP2	2.20	0.41
71:1:997:A:N6	71:1:1012:A:O5'	2.54	0.41
71:1:1080:A:H2'	71:1:1081:U:H6	1.85	0.41
71:1:1131:A:O5'	71:1:1131:A:H8	2.04	0.41
6:F:143:LEU:HD12	6:F:143:LEU:HA	1.92	0.41
7:G:211:VAL:O	7:G:211:VAL:HG13	2.20	0.41
10:J:54:ILE:HG23	10:J:120:GLY:CA	2.48	0.41
10:J:142:ARG:HB3	71:1:805:U:H5"	2.02	0.41
13:M:172:GLY:O	13:M:176:VAL:HG12	2.21	0.41
15:O:28:ALA:HB1	15:O:29:ARG:NE	2.23	0.41
18:R:312:THR:HG22	18:R:313:LYS:HG3	2.02	0.41
24:X:380:GLN:OE1	24:X:384:LYS:HD3	2.20	0.41
25:Y:101:GLU:OE2	25:Y:104:ARG:NH1	2.54	0.41
27:BA:104:LEU:HD23	27:BA:104:LEU:HA	1.96	0.41
50:BE:91:ILE:HG22	50:BE:95:ARG:HB2	2.03	0.41
61:BD:62:ARG:HA	61:BD:69:VAL:HA	2.02	0.41
65:BL:72:ARG:HA	65:BL:72:ARG:HD2	1.89	0.41
66:BO:49:ASN:OD1	66:BO:49:ASN:N	2.53	0.41
66:BO:50:GLY:HA2	66:BO:56:ALA:CB	2.49	0.41
66:BO:133:ARG:O	66:BO:147:PHE:HB2	2.21	0.41
67:BG:1288:PRO:C	67:BG:1290:CYS:H	2.24	0.41
71:1:649:A:O2'	71:1:650:U:OP2	2.38	0.41
71:1:688:C:H42	71:1:710:A:N6	2.18	0.41
1:A:185:VAL:HG23	10:J:20:PHE:CZ	2.55	0.41
1:A:234:GLY:HA3	29:BB:107:GLN:O	2.20	0.41
3:C:140:ASN:HB3	3:C:143:VAL:HG23	2.03	0.41
5:E:72:PHE:CG	5:E:79:ALA:HB2	2.55	0.41
5:E:179:ARG:HG3	5:E:179:ARG:NH1	2.32	0.41
7:G:87:ASN:O	7:G:90:ILE:HG12	2.21	0.41
7:G:189:LEU:HD23	7:G:189:LEU:HA	1.85	0.41
9:I:93:LEU:O	9:I:96:LEU:N	2.51	0.41
9:I:186:PHE:CZ	54:BF:21:VAL:HG21	2.55	0.41
14:N:170:ILE:O	14:N:219:LYS:HB3	2.21	0.41
18:R:220:SER:N	18:R:223:ASP:OD2	2.53	0.41
24:X:163:ALA:HA	24:X:409:CYS:O	2.21	0.41
26:Z:90:LEU:HA	26:Z:90:LEU:HD23	1.76	0.41
27:BA:66:ALA:CB	27:BA:87:ILE:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:93:HIS:NE2	52:BP:87:GLU:OE2	2.54	0.41
27:BA:145:ALA:O	27:BA:149:ALA:N	2.43	0.41
44:BM:76:TYR:CZ	44:BM:326:TYR:HB3	2.55	0.41
44:BM:137:ARG:NE	44:BM:278:LEU:HD12	2.35	0.41
44:BM:158:MET:SD	44:BM:214:LYS:HD3	2.60	0.41
44:BM:217:LYS:HB2	44:BM:217:LYS:HE3	1.88	0.41
52:BP:10:TYR:CE1	71:1:409:A:H1'	2.55	0.41
52:BP:94:ARG:HG3	52:BP:95:PRO:O	2.21	0.41
65:BL:98:MET:HE2	65:BL:98:MET:HB2	1.81	0.41
65:BL:127:LYS:HB2	71:1:667:A:OP1	2.20	0.41
68:UB:34:UNK:O	68:UB:36:UNK:N	2.53	0.41
71:1:610:A:H2'	71:1:611:A:O4'	2.21	0.41
1:A:262:VAL:HG22	71:1:809:A:C2	2.56	0.41
1:A:294:THR:N	10:J:6:GLU:OE2	2.53	0.41
2:B:216:VAL:O	2:B:329:THR:HA	2.21	0.41
2:B:242:HIS:ND1	13:M:59:ARG:HB3	2.36	0.41
2:B:243:LYS:HB3	2:B:243:LYS:HE2	1.90	0.41
6:F:113:ARG:H	6:F:113:ARG:HG3	1.52	0.41
9:I:45:MET:SD	68:UB:19:UNK:HA	2.61	0.41
9:I:153:ARG:HD2	9:I:158:VAL:CG1	2.50	0.41
10:J:5:ARG:NH1	71:1:1108:A:OP2	2.54	0.41
10:J:53:ILE:HD12	10:J:53:ILE:HA	1.83	0.41
16:P:26:ARG:HD3	71:1:340:U:OP1	2.20	0.41
17:Q:64:SER:OG	17:Q:81:ARG:HG3	2.21	0.41
18:R:261:ALA:HA	18:R:264:LEU:HG	2.02	0.41
20:T:38:LEU:HD21	71:1:533:U:H5"	2.02	0.41
26:Z:123:GLY:O	26:Z:131:TRP:HD1	2.03	0.41
29:BB:51:ALA:O	29:BB:55:GLN:NE2	2.53	0.41
44:BM:328:TYR:O	44:BM:331:PRO:HD2	2.20	0.41
52:BP:95:PRO:HA	52:BP:96:PRO:HD2	1.74	0.41
65:BL:247:LEU:HD13	65:BL:370:TYR:CE2	2.56	0.41
67:BG:1333:ILE:O	67:BG:1335:SER:N	2.54	0.41
71:1:178:U:H2'	71:1:327:U:O4	2.21	0.41
71:1:798:A:O2'	71:1:799:A:P	2.79	0.41
2:B:194:LYS:O	2:B:194:LYS:CE	2.68	0.41
5:E:55:PHE:HE1	5:E:71:GLU:OE2	2.03	0.41
5:E:302:THR:HG1	5:E:305:GLU:CD	2.24	0.41
13:M:13:ARG:NH2	71:1:506:A:O2'	2.52	0.41
13:M:159:ARG:NE	13:M:243:LEU:HD22	2.34	0.41
16:P:51:ARG:NE	16:P:53:PHE:CE2	2.89	0.41
16:P:86:VAL:HG11	16:P:110:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:107:GLY:O	17:Q:119:GLN:HA	2.21	0.41
18:R:116:ARG:HA	18:R:119:LYS:HB2	2.02	0.41
18:R:148:ARG:HB2	18:R:330:TRP:CE2	2.56	0.41
25:Y:220:TYR:HE1	37:BC:67:ASN:HD21	1.67	0.41
34:BI:96:VAL:HG22	34:BI:239:VAL:HG21	2.02	0.41
44:BM:22:THR:O	44:BM:24:PRO:HD3	2.21	0.41
44:BM:93:LEU:HA	44:BM:96:THR:OG1	2.20	0.41
44:BM:242:THR:HG1	44:BM:276:HIS:CE1	2.34	0.41
44:BM:258:ASP:C	44:BM:259:LYS:HD3	2.40	0.41
44:BM:268:HIS:O	44:BM:272:LYS:HG2	2.20	0.41
65:BL:90:PRO:O	65:BL:91:PHE:CB	2.68	0.41
65:BL:278:ARG:HD3	65:BL:278:ARG:C	2.40	0.41
66:BO:99:HIS:HB2	66:BO:128:VAL:HB	2.03	0.41
71:1:177:G:N2	71:1:525:U:H3	2.16	0.41
71:1:432:U:C2	71:1:433:G:C6	3.09	0.41
71:1:513:U:O2'	71:1:514:U:P	2.79	0.41
71:1:1004:U:H3'	71:1:1005:A:C8	2.55	0.41
71:1:1074:A:C1'	71:1:1075:A:P	3.08	0.41
2:B:69:GLU:OE2	2:B:69:GLU:N	2.52	0.41
7:G:34:LEU:HB3	7:G:37:GLU:HB2	2.01	0.41
7:G:329:PHE:CG	7:G:330:PRO:HD2	2.55	0.41
8:H:12:LEU:HG	8:H:12:LEU:O	2.21	0.41
8:H:55:ASP:OD1	8:H:152:GLN:HB3	2.20	0.41
8:H:61:GLN:HG2	8:H:114:TYR:CZ	2.56	0.41
9:I:72:ARG:HH22	71:1:544:U:P	2.43	0.41
9:I:256:GLU:HA	9:I:259:HIS:HD2	1.85	0.41
10:J:48:HIS:CE1	10:J:52:GLN:HG2	2.56	0.41
11:K:153:GLU:HB2	11:K:180:MET:SD	2.60	0.41
12:L:134:TYR:H	12:L:149:ASN:ND2	2.19	0.41
13:M:238:ASP:HB3	13:M:241:MET:HB2	2.03	0.41
16:P:165:PRO:HA	16:P:176:LEU:HD11	2.03	0.41
18:R:429:VAL:O	18:R:433:VAL:HG12	2.21	0.41
19:S:294:ILE:HG13	19:S:296:PRO:HD2	2.02	0.41
22:V:58:LEU:HD23	22:V:58:LEU:HA	1.54	0.41
24:X:302:THR:C	24:X:305:GLY:H	2.24	0.41
25:Y:87:GLU:O	25:Y:91:ARG:HG2	2.20	0.41
34:BI:239:VAL:HA	34:BI:242:ALA:HB3	2.03	0.41
44:BM:171:ASP:OD1	44:BM:172:ALA:N	2.54	0.41
44:BM:380:THR:HG22	44:BM:384:HIS:CE1	2.56	0.41
47:BH:33:ILE:HD12	47:BH:43:VAL:HG21	2.01	0.41
47:BH:148:ARG:HA	47:BH:148:ARG:HD2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BP:97:ARG:H	52:BP:98:PRO:HD2	1.75	0.41
65:BL:205:LEU:HD22	65:BL:210:GLN:CD	2.41	0.41
65:BL:214:LEU:O	65:BL:217:VAL:HG22	2.21	0.41
66:BO:70:ASP:HB2	66:BO:163:GLY:HA3	2.03	0.41
67:BG:1340:GLU:OE2	67:BG:1343:ASN:HB2	2.20	0.41
71:1:542:G:N3	71:1:596:U:O2'	2.51	0.41
71:1:641:A:H2	71:1:798:A:N6	2.18	0.41
71:1:879:A:H8	71:1:879:A:O5'	2.04	0.41
1:A:143:ASP:HB3	1:A:307:TRP:HE1	1.86	0.41
1:A:302:ASP:O	1:A:335:THR:OG1	2.39	0.41
2:B:125:LEU:HD11	2:B:129:LEU:HD21	2.03	0.41
2:B:251:ASP:HB2	2:B:278:LEU:HD11	2.03	0.41
2:B:434:MET:CG	7:G:275:MET:HB3	2.51	0.41
5:E:49:VAL:HG21	5:E:52:ASN:ND2	2.36	0.41
5:E:264:LEU:HD21	5:E:295:ARG:HG3	2.03	0.41
6:F:100:TRP:CZ2	6:F:122:LEU:HB3	2.56	0.41
7:G:54:ARG:HD3	7:G:63:LEU:HD22	2.03	0.41
7:G:70:LEU:HG	71:1:498:G:OP2	2.21	0.41
7:G:237:ALA:HB3	7:G:242:ILE:HG13	2.02	0.41
8:H:11:LEU:HD23	8:H:11:LEU:N	2.36	0.41
12:L:57:LYS:HE2	52:BP:19:ILE:O	2.21	0.41
13:M:32:TYR:CD1	71:1:176:A:H4'	2.55	0.41
13:M:62:LEU:HD23	13:M:91:ARG:HG2	2.02	0.41
13:M:99:LEU:CD2	13:M:108:GLN:HA	2.51	0.41
13:M:143:TRP:HB3	15:O:36:PHE:CE2	2.55	0.41
17:Q:50:ASN:O	17:Q:53:ALA:N	2.54	0.41
18:R:48:GLN:H	18:R:48:GLN:HG2	1.73	0.41
21:U:68:LEU:H	21:U:85:GLU:HG2	1.85	0.41
22:V:51:PHE:H	22:V:53:ARG:NH1	2.19	0.41
22:V:104:ARG:NE	71:1:184:G:C8	2.88	0.41
24:X:379:LYS:NZ	24:X:382:GLY:HA3	2.36	0.41
25:Y:177:PHE:C	25:Y:179:TYR:H	2.23	0.41
27:BA:39:ALA:HB1	27:BA:124:VAL:HG23	2.03	0.41
29:BB:92:ASN:OD1	29:BB:93:THR:N	2.51	0.41
29:BB:127:PRO:HB3	50:BE:43:GLU:HG2	2.03	0.41
34:BI:197:LEU:HD12	34:BI:232:ARG:HB3	2.03	0.41
34:BI:249:THR:OG1	34:BI:250:ALA:N	2.53	0.41
44:BM:244:LEU:O	44:BM:247:PHE:HB3	2.21	0.41
47:BH:186:ARG:NH1	47:BH:225:ILE:O	2.54	0.41
47:BH:223:ASP:C	47:BH:224:LEU:HD22	2.41	0.41
52:BP:24:TYR:O	52:BP:27:GLY:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BL:247:LEU:HD23	65:BL:247:LEU:HA	1.65	0.41
65:BL:337:ARG:NE	65:BL:337:ARG:HA	2.35	0.41
66:BO:81:ALA:HA	66:BO:99:HIS:CD2	2.55	0.41
66:BO:87:ARG:CB	66:BO:90:HIS:HB3	2.44	0.41
70:UD:26:UNK:C	70:UD:28:UNK:N	2.83	0.41
71:1:74:A:HO2'	71:1:75:A:P	2.44	0.41
71:1:149:U:O2'	71:1:150:A:H8	2.04	0.41
71:1:163:U:H3	71:1:1013:U:H5'	1.84	0.41
71:1:302:A:N6	71:1:303:U:O4	2.54	0.41
71:1:391:A:O3'	71:1:392:A:H3'	2.21	0.41
71:1:393:A:O2'	71:1:394:U:P	2.79	0.41
71:1:465:A:N6	71:1:466:U:C4	2.89	0.41
71:1:628:U:H4'	71:1:629:A:OP1	2.19	0.41
71:1:648:U:O2'	71:1:649:A:OP2	2.38	0.41
71:1:652:A:C8	71:1:758:G:O6	2.74	0.41
71:1:810:U:C3'	71:1:811:U:H5"	2.51	0.41
71:1:911:A:C6	71:1:912:U:C4	3.09	0.41
71:1:975:U:N3	71:1:976:A:H2	2.18	0.41
1:A:83:GLN:HB2	50:BE:114:LEU:O	2.20	0.41
2:B:174:TRP:HA	22:V:13:GLY:HA2	2.03	0.41
2:B:284:LEU:HD23	2:B:339:GLU:CD	2.41	0.41
7:G:157:VAL:CG2	22:V:58:LEU:HD12	2.48	0.41
9:I:88:ALA:HB2	71:1:600:A:C8	2.56	0.41
12:L:88:ARG:HB3	12:L:110:GLN:HB2	2.03	0.41
13:M:29:GLN:HG2	13:M:30:LYS:H	1.86	0.41
13:M:62:LEU:HD22	13:M:84:GLU:HG3	2.02	0.41
15:O:141:THR:OG1	15:O:203:VAL:O	2.18	0.41
15:O:176:VAL:HB	15:O:189:VAL:O	2.21	0.41
16:P:51:ARG:C	16:P:60:ARG:HD3	2.42	0.41
17:Q:197:LEU:HA	17:Q:200:VAL:HG12	2.03	0.41
19:S:334:ALA:C	19:S:336:GLN:H	2.24	0.41
22:V:116:ASP:OD1	22:V:117:ILE:N	2.54	0.41
25:Y:220:TYR:CE1	37:BC:67:ASN:ND2	2.89	0.41
26:Z:107:PHE:CE1	26:Z:112:PRO:HA	2.56	0.41
27:BA:112:GLU:HA	27:BA:137:ARG:O	2.21	0.41
29:BB:69:SER:OG	29:BB:73:GLU:HG3	2.21	0.41
52:BP:2:LEU:HD13	52:BP:2:LEU:HA	1.92	0.41
66:BO:188:PHE:CD1	66:BO:188:PHE:C	2.94	0.41
67:BG:1327:LYS:HA	67:BG:1327:LYS:HD2	1.88	0.41
71:1:252:U:C4	71:1:253:U:C2	3.09	0.41
71:1:544:U:H1'	71:1:595:A:C2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1:594:U:O2'	71:1:595:A:P	2.79	0.41
1:A:281:GLN:HB2	1:A:283:ARG:HG2	2.03	0.40
1:A:383:PHE:CE1	10:J:110:LYS:HD2	2.56	0.40
5:E:171:PRO:HD2	5:E:176:ARG:HH11	1.84	0.40
7:G:218:LEU:O	7:G:219:LEU:HD23	2.21	0.40
11:K:158:ARG:HH21	52:BP:-41:ARG:HG2	1.86	0.40
14:N:138:PHE:HA	14:N:141:PHE:HB3	2.03	0.40
17:Q:30:LEU:O	17:Q:33:ARG:HB3	2.20	0.40
17:Q:122:MET:HE2	17:Q:122:MET:HB2	1.67	0.40
25:Y:74:TYR:O	25:Y:77:TYR:N	2.54	0.40
25:Y:223:LEU:HA	25:Y:223:LEU:HD23	1.90	0.40
34:BI:198:LEU:HD11	34:BI:212:PHE:HB2	2.03	0.40
44:BM:134:LYS:HA	44:BM:134:LYS:HD3	1.87	0.40
44:BM:298:ALA:O	44:BM:302:MET:HB2	2.20	0.40
61:BD:29:ILE:HG12	61:BD:30:ALA:O	2.21	0.40
66:BO:36:ILE:N	71:1:1128:U:O2	2.54	0.40
71:1:542:G:C2	71:1:596:U:C6	3.09	0.40
71:1:643:G:C5'	71:1:656:G:H22	2.34	0.40
71:1:828:A:N3	71:1:828:A:H2'	2.36	0.40
71:1:923:A:C2	71:1:980:A:N7	2.89	0.40
71:1:936:G:N2	71:1:937:C:C2	2.89	0.40
1:A:173:VAL:O	1:A:175:THR:HG23	2.22	0.40
1:A:384:ARG:NH2	71:1:1149:A:OP1	2.54	0.40
2:B:127:TYR:OH	2:B:310:ILE:HG12	2.21	0.40
2:B:146:ILE:HD13	2:B:146:ILE:HA	1.77	0.40
9:I:11:ARG:NH2	66:BO:53:GLY:HA2	2.36	0.40
9:I:65:HIS:O	9:I:69:ILE:HG13	2.21	0.40
9:I:219:GLU:HA	9:I:222:HIS:HB3	2.03	0.40
14:N:71:TRP:CD1	71:1:315:A:H1'	2.56	0.40
15:O:138:PRO:HA	15:O:156:ILE:HG22	2.02	0.40
18:R:243:ILE:HD11	18:R:258:VAL:N	2.36	0.40
18:R:362:GLU:H	18:R:362:GLU:HG2	1.41	0.40
24:X:245:ASP:HA	24:X:250:GLN:HE21	1.86	0.40
25:Y:96:MET:HE2	37:BC:22:HIS:HB3	2.03	0.40
27:BA:23:TYR:O	27:BA:26:LYS:N	2.54	0.40
34:BI:173:GLN:HE22	34:BI:202:VAL:HA	1.86	0.40
34:BI:193:ASP:OD1	34:BI:193:ASP:N	2.54	0.40
47:BH:190:SER:HB2	47:BH:223:ASP:HA	2.03	0.40
50:BE:88:GLU:HG3	50:BE:90:GLU:OE2	2.21	0.40
61:BD:20:GLN:HB3	61:BD:64:HIS:HD2	1.86	0.40
65:BL:257:LEU:HD12	65:BL:267:PHE:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:BO:73:ASN:HB2	66:BO:119:ARG:HE	1.86	0.40
66:BO:81:ALA:HB1	66:BO:86:GLU:OE2	2.21	0.40
69:UC:121:UNK:C	69:UC:123:UNK:N	2.83	0.40
71:1:228:G:C2	71:1:310:A:C2	3.09	0.40
71:1:236:A:H1'	71:1:288:C:N4	2.32	0.40
71:1:476:A:O2'	71:1:477:U:OP1	2.33	0.40
71:1:712:U:OP2	71:1:749:U:H5"	2.21	0.40
71:1:780:U:C4	71:1:781:A:C6	3.09	0.40
71:1:798:A:C2	71:1:799:A:C6	3.09	0.40
71:1:821:U:H2'	71:1:822:A:O4'	2.22	0.40
71:1:1033:U:H2'	71:1:1034:C:N1	2.36	0.40
71:1:1075:A:C2	71:1:1092:G:C2	3.10	0.40
71:1:1080:A:H8	71:1:1088:G:N2	2.20	0.40
1:A:387:PHE:CD1	1:A:387:PHE:N	2.89	0.40
2:B:201:ARG:HA	2:B:204:VAL:HG12	2.02	0.40
3:C:69:THR:HG23	3:C:69:THR:O	2.21	0.40
3:C:132:ARG:HE	3:C:132:ARG:HB3	1.60	0.40
4:D:59:ASP:N	4:D:60:PRO:HD2	2.35	0.40
5:E:119:PRO:HD2	5:E:124:PHE:CZ	2.57	0.40
6:F:54:ILE:HB	6:F:127:LEU:HD13	2.03	0.40
7:G:356:LEU:HA	7:G:356:LEU:HD23	1.80	0.40
11:K:31:GLU:HB2	11:K:34:VAL:CG1	2.50	0.40
13:M:214:ASP:HB2	13:M:224:LYS:HG3	2.02	0.40
14:N:122:PRO:HG3	18:R:460:HIS:HB2	2.03	0.40
15:O:35:ARG:HH12	71:1:43:A:H3'	1.85	0.40
15:O:184:ARG:HH22	15:O:187:GLN:HE21	1.69	0.40
16:P:164:ASP:OD2	16:P:166:ASN:HB2	2.20	0.40
19:S:348:ALA:HA	71:1:368:U:C6	2.56	0.40
22:V:104:ARG:NH2	71:1:184:G:OP2	2.46	0.40
24:X:261:PHE:HE1	24:X:339:CYS:HB3	1.85	0.40
24:X:498:ARG:HA	24:X:498:ARG:HD3	1.91	0.40
27:BA:49:SER:O	27:BA:53:LYS:N	2.46	0.40
27:BA:82:LEU:HD13	27:BA:146:VAL:HG23	2.03	0.40
27:BA:91:HIS:CG	27:BA:92:PRO:HD2	2.55	0.40
44:BM:97:GLY:HA2	44:BM:100:ALA:HB3	2.03	0.40
44:BM:129:LEU:HD13	44:BM:129:LEU:HA	1.92	0.40
44:BM:373:LYS:HA	44:BM:376:ILE:HG12	2.03	0.40
47:BH:132:HIS:HB2	47:BH:137:GLN:O	2.21	0.40
65:BL:179:ASN:O	65:BL:180:GLY:C	2.60	0.40
65:BL:263:GLU:HB2	65:BL:352:ARG:O	2.21	0.40
65:BL:305:HIS:HE1	71:1:678:U:OP2	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:BG:1338:LEU:H	67:BG:1338:LEU:HG	1.65	0.40
68:UB:59:UNK:O	68:UB:63:UNK:N	2.54	0.40
71:1:229:A:C8	71:1:290:C:N4	2.89	0.40
71:1:396:A:N6	71:1:397:A:C5	2.90	0.40
71:1:862:A:H2'	71:1:863:A:O4'	2.21	0.40
71:1:998:G:N3	71:1:998:G:H2'	2.37	0.40
71:1:1103:U:C4	71:1:1104:U:C2	3.10	0.40
71:1:1105:G:OP2	71:1:1105:G:C8	2.73	0.40
1:A:283:ARG:CD	71:1:840:A:H5"	2.49	0.40
1:A:356:PHE:HA	29:BB:98:THR:OG1	2.22	0.40
2:B:75:THR:HB	2:B:77:ARG:O	2.22	0.40
3:C:31:GLU:OE2	3:C:74:SER:HB2	2.21	0.40
5:E:21:PRO:O	5:E:224:GLN:NE2	2.51	0.40
7:G:145:ARG:HD2	71:1:346:A:H5"	2.04	0.40
7:G:148:THR:O	7:G:149:PRO:C	2.60	0.40
7:G:228:TYR:CE1	7:G:230:LEU:HD13	2.56	0.40
9:I:114:GLN:NE2	68:UB:19:UNK:O	2.54	0.40
12:L:109:ALA:HB2	71:1:405:U:O2'	2.22	0.40
14:N:112:VAL:HG13	14:N:121:TRP:CZ3	2.57	0.40
14:N:166:PRO:O	14:N:223:VAL:HG12	2.21	0.40
17:Q:13:PHE:HB2	17:Q:16:ASN:OD1	2.22	0.40
18:R:70:ARG:HD3	18:R:70:ARG:HA	1.94	0.40
21:U:28:LYS:HA	21:U:28:LYS:HZ2	1.86	0.40
22:V:32:PHE:HZ	71:1:91:U:C5	2.40	0.40
22:V:95:LEU:HD22	22:V:108:MET:HE2	2.04	0.40
24:X:234:ALA:N	24:X:237:ALA:HA	2.36	0.40
44:BM:7:LEU:O	44:BM:11:VAL:HG22	2.21	0.40
44:BM:214:LYS:HD2	44:BM:214:LYS:HA	1.81	0.40
44:BM:247:PHE:HD2	44:BM:248:THR:HG23	1.87	0.40
47:BH:49:ARG:NH2	47:BH:198:TYR:HD2	2.19	0.40
65:BL:135:ARG:HD3	71:1:235:G:OP1	2.22	0.40
65:BL:155:ILE:HG21	65:BL:179:ASN:OD1	2.21	0.40
65:BL:341:LYS:HE2	65:BL:341:LYS:HB3	1.87	0.40
71:1:226:A:H61	71:1:310:A:H62	1.69	0.40
71:1:412:U:H6	71:1:412:U:H2'	1.76	0.40
71:1:608:A:H1'	71:1:817:A:H61	1.85	0.40
71:1:656:G:N7	71:1:679:A:N6	2.69	0.40
71:1:950:A:O2'	71:1:951:U:H5"	2.21	0.40
71:1:971:U:H4'	71:1:972:A:OP2	2.21	0.40
1:A:129:VAL:CG1	1:A:333:ARG:HH12	2.35	0.40
2:B:179:LYS:NZ	71:1:215:U:O3'	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:LEU:C	2:B:258:PRO:HD3	2.41	0.40
4:D:30:LEU:HA	4:D:39:GLN:O	2.21	0.40
5:E:129:ILE:HG22	5:E:149:LEU:HD21	2.03	0.40
8:H:45:ILE:HD13	8:H:156:VAL:HG23	2.04	0.40
9:I:57:LYS:HG3	9:I:57:LYS:O	2.20	0.40
11:K:137:ARG:HE	11:K:146:PRO:HD3	1.85	0.40
14:N:105:ILE:HG12	26:Z:86:ILE:HD13	2.03	0.40
16:P:33:HIS:ND1	16:P:45:LYS:HE2	2.37	0.40
17:Q:158:ARG:HA	17:Q:158:ARG:HD3	1.74	0.40
18:R:57:GLU:HG3	26:Z:155:PRO:HG3	2.03	0.40
18:R:104:GLU:OE2	18:R:104:GLU:HA	2.21	0.40
25:Y:224:HIS:HD2	37:BC:66:LEU:HD22	1.87	0.40
44:BM:31:ARG:HD2	44:BM:31:ARG:HA	1.89	0.40
54:BF:93:LYS:NZ	71:1:562:U:H5"	2.36	0.40
65:BL:263:GLU:OE1	65:BL:353:GLY:HA2	2.22	0.40
71:1:51:U:O4	71:1:119:G:N2	2.54	0.40
71:1:166:U:H1'	71:1:847:A:N6	2.37	0.40
71:1:205:U:C2'	71:1:206:U:H5'	2.52	0.40
71:1:419:U:C2	71:1:420:A:N6	2.89	0.40
71:1:912:U:O4	71:1:913:A:C5	2.74	0.40
71:1:982:A:O2'	71:1:983:U:H5"	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	366/467 (78%)	315 (86%)	48 (13%)	3 (1%)	19 59
2	B	433/436 (99%)	380 (88%)	52 (12%)	1 (0%)	47 79
3	C	210/262 (80%)	179 (85%)	31 (15%)	0	100 100
4	D	126/204 (62%)	108 (86%)	18 (14%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	324/346 (94%)	294 (91%)	30 (9%)	0	100	100
6	F	168/171 (98%)	152 (90%)	15 (9%)	1 (1%)	25	64
7	G	363/374 (97%)	313 (86%)	48 (13%)	2 (1%)	25	64
8	H	160/168 (95%)	144 (90%)	14 (9%)	2 (1%)	12	50
9	I	255/305 (84%)	224 (88%)	31 (12%)	0	100	100
10	J	139/144 (96%)	102 (73%)	36 (26%)	1 (1%)	22	61
11	K	177/194 (91%)	158 (89%)	19 (11%)	0	100	100
12	L	176/186 (95%)	157 (89%)	18 (10%)	1 (1%)	25	64
13	M	257/279 (92%)	217 (84%)	39 (15%)	1 (0%)	34	71
14	N	187/252 (74%)	163 (87%)	24 (13%)	0	100	100
15	O	305/476 (64%)	271 (89%)	29 (10%)	5 (2%)	9	46
16	P	163/185 (88%)	145 (89%)	17 (10%)	1 (1%)	25	64
17	Q	215/234 (92%)	192 (89%)	22 (10%)	1 (0%)	29	68
18	R	470/480 (98%)	409 (87%)	60 (13%)	1 (0%)	47	79
19	S	148/409 (36%)	132 (89%)	16 (11%)	0	100	100
20	T	53/83 (64%)	50 (94%)	3 (6%)	0	100	100
21	U	90/118 (76%)	75 (83%)	13 (14%)	2 (2%)	6	39
22	V	139/151 (92%)	119 (86%)	20 (14%)	0	100	100
23	W	52/186 (28%)	46 (88%)	6 (12%)	0	100	100
24	X	466/513 (91%)	418 (90%)	45 (10%)	3 (1%)	25	64
25	Y	253/292 (87%)	234 (92%)	19 (8%)	0	100	100
26	Z	148/197 (75%)	117 (79%)	28 (19%)	3 (2%)	7	41
27	BA	136/167 (81%)	103 (76%)	29 (21%)	4 (3%)	4	33
29	BB	120/156 (77%)	95 (79%)	23 (19%)	2 (2%)	9	45
30	Aw	183/187 (98%)	161 (88%)	22 (12%)	0	100	100
31	Bj	166/185 (90%)	143 (86%)	22 (13%)	1 (1%)	25	64
32	An	312/331 (94%)	256 (82%)	49 (16%)	7 (2%)	6	39
33	Al	262/346 (76%)	219 (84%)	43 (16%)	0	100	100
34	BI	184/266 (69%)	155 (84%)	29 (16%)	0	100	100
35	Az	136/152 (90%)	109 (80%)	25 (18%)	2 (2%)	10	47
36	At	163/183 (89%)	145 (89%)	18 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BC	138/147 (94%)	127 (92%)	11 (8%)	0	100	100
38	Ab	258/262 (98%)	226 (88%)	32 (12%)	0	100	100
39	Ai	474/479 (99%)	413 (87%)	60 (13%)	1 (0%)	47	79
40	Ap	212/240 (88%)	188 (89%)	24 (11%)	0	100	100
41	Au	174/186 (94%)	132 (76%)	36 (21%)	6 (3%)	3	31
42	Aa	176/195 (90%)	142 (81%)	32 (18%)	2 (1%)	14	53
43	Ao	273/284 (96%)	233 (85%)	38 (14%)	2 (1%)	22	61
44	BM	387/457 (85%)	326 (84%)	61 (16%)	0	100	100
45	Ar	193/205 (94%)	167 (86%)	26 (14%)	0	100	100
46	Aj	337/503 (67%)	292 (87%)	45 (13%)	0	100	100
47	BH	212/229 (93%)	185 (87%)	27 (13%)	0	100	100
48	Am	328/340 (96%)	275 (84%)	53 (16%)	0	100	100
49	Aq	250/341 (73%)	199 (80%)	45 (18%)	6 (2%)	6	37
50	BE	82/118 (70%)	56 (68%)	25 (30%)	1 (1%)	13	51
51	Ak	298/323 (92%)	254 (85%)	44 (15%)	0	100	100
52	BP	191/254 (75%)	162 (85%)	28 (15%)	1 (0%)	29	68
53	Ad	203/237 (86%)	163 (80%)	38 (19%)	2 (1%)	15	55
54	BF	99/109 (91%)	79 (80%)	20 (20%)	0	100	100
55	Av	153/192 (80%)	128 (84%)	25 (16%)	0	100	100
56	Af	137/155 (88%)	119 (87%)	18 (13%)	0	100	100
57	As	95/249 (38%)	87 (92%)	8 (8%)	0	100	100
58	Ae	289/311 (93%)	253 (88%)	36 (12%)	0	100	100
59	Ac	266/291 (91%)	234 (88%)	32 (12%)	0	100	100
60	Ah	450/570 (79%)	386 (86%)	62 (14%)	2 (0%)	34	71
61	BD	95/102 (93%)	85 (90%)	10 (10%)	0	100	100
62	Ay	140/174 (80%)	117 (84%)	18 (13%)	5 (4%)	3	29
63	Ag	229/244 (94%)	204 (89%)	25 (11%)	0	100	100
64	Ax	165/216 (76%)	134 (81%)	31 (19%)	0	100	100
65	BL	307/380 (81%)	235 (76%)	66 (22%)	6 (2%)	7	41
66	BO	153/190 (80%)	105 (69%)	45 (29%)	3 (2%)	7	41
67	BG	83/1347 (6%)	57 (69%)	23 (28%)	3 (4%)	3	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	14352/18415 (78%)	12263 (85%)	2005 (14%)	84 (1%)	29 64

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	ILE
6	F	167	ASN
8	H	94	VAL
10	J	66	PRO
21	U	30	ILE
24	X	353	PRO
26	Z	26	HIS
27	BA	24	VAL
29	BB	110	PHE
32	An	46	GLN
32	An	50	HIS
32	An	97	SER
41	Au	54	PRO
42	Aa	191	THR
49	Aq	172	ILE
49	Aq	175	VAL
62	Ay	36	ILE
62	Ay	164	ARG
65	BL	115	TYR
66	BO	184	VAL
67	BG	1265	PRO
7	G	149	PRO
7	G	159	ALA
15	O	20	THR
15	O	21	TYR
15	O	28	ALA
15	O	31	ARG
24	X	355	THR
26	Z	44	LEU
26	Z	106	TYR
35	Az	16	LYS
41	Au	27	GLU
41	Au	92	VAL
41	Au	93	HIS
42	Aa	189	ARG
43	Ao	20	VAL
49	Aq	338	HIS

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Mol	Chain	Res	Type
50	BE	37	GLU
52	BP	96	PRO
60	Ah	67	ARG
66	BO	92	ARG
18	R	137	PRO
27	BA	114	PHE
29	BB	129	THR
35	Az	17	GLN
41	Au	96	LEU
49	Aq	53	SER
49	Aq	168	GLN
53	Ad	15	PRO
53	Ad	27	HIS
62	Ay	35	TRP
67	BG	1263	HIS
21	U	29	VAL
31	Bj	76	PRO
32	An	44	TRP
41	Au	45	THR
43	Ao	19	ARG
62	Ay	166	GLN
15	O	27	TYR
16	P	56	ASP
17	Q	90	ARG
27	BA	23	TYR
32	An	77	TRP
32	An	215	VAL
65	BL	116	PHE
66	BO	61	SER
12	L	72	PRO
27	BA	45	GLN
32	An	142	GLY
1	A	159	PRO
1	A	377	PRO
24	X	364	PRO
39	Ai	161	PRO
62	Ay	168	TRP
65	BL	74	PRO
65	BL	324	PRO
65	BL	340	VAL
67	BG	1318	PRO
2	B	302	GLY

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Mol	Chain	Res	Type
8	H	93	VAL
13	M	14	PRO
65	BL	311	VAL
49	Aq	54	ILE
60	Ah	64	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	314/394 (80%)	313 (100%)	1 (0%)	92 97
2	B	380/381 (100%)	375 (99%)	5 (1%)	69 86
3	C	190/227 (84%)	190 (100%)	0	100 100
4	D	106/154 (69%)	104 (98%)	2 (2%)	57 80
5	E	285/301 (95%)	270 (95%)	15 (5%)	22 58
6	F	151/152 (99%)	149 (99%)	2 (1%)	69 86
7	G	315/323 (98%)	305 (97%)	10 (3%)	39 70
8	H	138/143 (96%)	137 (99%)	1 (1%)	84 93
9	I	223/262 (85%)	221 (99%)	2 (1%)	78 90
10	J	119/122 (98%)	115 (97%)	4 (3%)	37 69
11	K	151/162 (93%)	149 (99%)	2 (1%)	69 86
12	L	151/158 (96%)	151 (100%)	0	100 100
13	M	226/242 (93%)	222 (98%)	4 (2%)	59 81
14	N	175/220 (80%)	172 (98%)	3 (2%)	60 82
15	O	278/397 (70%)	272 (98%)	6 (2%)	52 77
16	P	147/163 (90%)	147 (100%)	0	100 100
17	Q	191/204 (94%)	189 (99%)	2 (1%)	76 88
18	R	406/412 (98%)	403 (99%)	3 (1%)	84 93
19	S	135/336 (40%)	135 (100%)	0	100 100
20	T	52/74 (70%)	52 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	80/100 (80%)	75 (94%)	5 (6%)	18	53
22	V	125/135 (93%)	120 (96%)	5 (4%)	31	65
23	W	50/164 (30%)	46 (92%)	4 (8%)	12	43
24	X	402/438 (92%)	395 (98%)	7 (2%)	60	82
25	Y	209/236 (89%)	207 (99%)	2 (1%)	76	88
26	Z	132/172 (77%)	128 (97%)	4 (3%)	41	71
27	BA	112/135 (83%)	108 (96%)	4 (4%)	35	67
29	BB	106/140 (76%)	103 (97%)	3 (3%)	43	72
30	Aw	157/159 (99%)	156 (99%)	1 (1%)	86	94
31	Bj	150/165 (91%)	149 (99%)	1 (1%)	84	93
32	An	274/289 (95%)	265 (97%)	9 (3%)	38	69
33	Al	236/299 (79%)	230 (98%)	6 (2%)	47	75
34	BI	153/221 (69%)	152 (99%)	1 (1%)	84	93
35	Az	129/143 (90%)	126 (98%)	3 (2%)	50	76
36	At	140/153 (92%)	140 (100%)	0	100	100
37	BC	117/124 (94%)	116 (99%)	1 (1%)	78	90
38	Ab	233/235 (99%)	233 (100%)	0	100	100
39	Ai	408/410 (100%)	406 (100%)	2 (0%)	88	95
40	Ap	189/208 (91%)	188 (100%)	1 (0%)	88	95
41	Au	154/164 (94%)	145 (94%)	9 (6%)	20	55
42	Aa	150/166 (90%)	145 (97%)	5 (3%)	38	69
43	Ao	236/245 (96%)	234 (99%)	2 (1%)	81	91
44	BM	319/370 (86%)	315 (99%)	4 (1%)	69	86
45	Ar	169/179 (94%)	168 (99%)	1 (1%)	86	94
46	Aj	286/420 (68%)	284 (99%)	2 (1%)	84	93
47	BH	177/189 (94%)	175 (99%)	2 (1%)	73	88
48	Am	278/287 (97%)	276 (99%)	2 (1%)	84	93
49	Aq	221/276 (80%)	216 (98%)	5 (2%)	50	76
50	BE	76/100 (76%)	75 (99%)	1 (1%)	69	86
51	Ak	254/272 (93%)	252 (99%)	2 (1%)	81	91
52	BP	167/215 (78%)	165 (99%)	2 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
53	Ad	172/193 (89%)	171 (99%)	1 (1%)	86 94
54	BF	88/95 (93%)	87 (99%)	1 (1%)	73 88
55	Av	141/169 (83%)	141 (100%)	0	100 100
56	Af	120/135 (89%)	120 (100%)	0	100 100
57	As	88/204 (43%)	88 (100%)	0	100 100
58	Ae	249/261 (95%)	244 (98%)	5 (2%)	55 79
59	Ac	232/253 (92%)	230 (99%)	2 (1%)	78 90
60	Ah	385/485 (79%)	376 (98%)	9 (2%)	50 76
61	BD	85/90 (94%)	83 (98%)	2 (2%)	49 75
62	Ay	130/158 (82%)	128 (98%)	2 (2%)	65 84
63	Ag	202/211 (96%)	199 (98%)	3 (2%)	65 84
64	Ax	150/190 (79%)	141 (94%)	9 (6%)	19 54
65	BL	268/329 (82%)	261 (97%)	7 (3%)	46 74
66	BO	130/158 (82%)	125 (96%)	5 (4%)	33 66
67	BG	67/1047 (6%)	65 (97%)	2 (3%)	41 71
All	All	12529/15614 (80%)	12323 (98%)	206 (2%)	64 83

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
2	B	131	ARG
2	B	192	ASP
2	B	193	VAL
2	B	194	LYS
2	B	403	PRO
4	D	68	ASP
4	D	87	TYR
5	E	25	ARG
5	E	115	ARG
5	E	148	TYR
5	E	169	GLU
5	E	170	TYR
5	E	173	ILE
5	E	175	VAL
5	E	177	VAL
5	E	233	LEU

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Mol	Chain	Res	Type
5	E	240	GLU
5	E	263	ASN
5	E	277	LEU
5	E	286	GLU
5	E	320	ASP
5	E	322	GLN
6	F	157	ASP
6	F	161	GLN
7	G	142	TRP
7	G	143	GLN
7	G	145	ARG
7	G	146	LYS
7	G	149	PRO
7	G	150	ARG
7	G	153	LEU
7	G	212	VAL
7	G	235	GLN
7	G	358	TRP
8	H	24	ARG
9	I	21	ARG
9	I	186	PHE
10	J	21	PHE
10	J	46	TRP
10	J	66	PRO
10	J	67	ARG
11	K	12	ARG
11	K	29	ARG
13	M	9	ASN
13	M	14	PRO
13	M	54	MET
13	M	56	SER
14	N	85	ARG
14	N	173	ASP
14	N	198	ARG
15	O	19	PHE
15	O	20	THR
15	O	29	ARG
15	O	30	TYR
15	O	58	LYS
15	O	230	ARG
17	Q	28	ARG
17	Q	42	TRP

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Mol	Chain	Res	Type
18	R	138	THR
18	R	362	GLU
18	R	438	ARG
21	U	17	ARG
21	U	19	LYS
21	U	28	LYS
21	U	30	ILE
21	U	36	ASN
22	V	11	LYS
22	V	39	VAL
22	V	54	VAL
22	V	66	ARG
22	V	81	ARG
23	W	72	HIS
23	W	74	GLU
23	W	94	LYS
23	W	97	ASN
24	X	264	LEU
24	X	270	TYR
24	X	283	ARG
24	X	326	PRO
24	X	353	PRO
24	X	497	SER
24	X	498	ARG
25	Y	58	ARG
25	Y	160	LEU
26	Z	40	THR
26	Z	43	ILE
26	Z	44	LEU
26	Z	45	ARG
27	BA	23	TYR
27	BA	113	MET
27	BA	115	VAL
27	BA	127	CYS
29	BB	44	LYS
29	BB	110	PHE
29	BB	111	PHE
30	Aw	6	VAL
31	Bj	143	ASN
32	An	76	LYS
32	An	101	ILE
32	An	106	TRP

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Mol	Chain	Res	Type
32	An	129	LYS
32	An	140	ARG
32	An	143	TYR
32	An	217	ARG
32	An	221	GLN
32	An	255	VAL
33	Al	39	GLN
33	Al	268	TYR
33	Al	269	GLU
33	Al	274	VAL
33	Al	279	ASN
33	Al	287	TRP
34	BI	165	ILE
35	Az	35	LEU
35	Az	60	HIS
35	Az	93	LYS
37	BC	68	ASP
39	Ai	72	ARG
39	Ai	133	MET
40	Ap	173	ARG
41	Au	44	ARG
41	Au	46	VAL
41	Au	47	LEU
41	Au	51	PHE
41	Au	71	MET
41	Au	72	ASP
41	Au	77	VAL
41	Au	93	HIS
41	Au	117	ARG
42	Aa	39	TYR
42	Aa	46	MET
42	Aa	75	ARG
42	Aa	81	ASN
42	Aa	91	LEU
43	Ao	27	ARG
43	Ao	33	LEU
44	BM	17	ARG
44	BM	134	LYS
44	BM	138	VAL
44	BM	263	ARG
45	Ar	69	CYS
46	Aj	133	ARG

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Mol	Chain	Res	Type
46	Aj	391	LYS
47	BH	54	ARG
47	BH	225	ILE
48	Am	14	THR
48	Am	332	THR
49	Aq	174	ARG
49	Aq	176	ARG
49	Aq	336	ARG
49	Aq	339	ARG
49	Aq	341	PHE
50	BE	67	LYS
51	Ak	44	ARG
51	Ak	241	ARG
52	BP	0	TRP
52	BP	9	ARG
53	Ad	32	ARG
54	BF	103	HIS
58	Ae	89	ASP
58	Ae	95	ARG
58	Ae	163	VAL
58	Ae	254	ASP
58	Ae	286	LYS
59	Ac	47	ARG
59	Ac	278	LYS
60	Ah	57	LEU
60	Ah	58	VAL
60	Ah	67	ARG
60	Ah	68	ILE
60	Ah	112	TYR
60	Ah	165	TYR
60	Ah	182	ARG
60	Ah	279	ASP
60	Ah	357	LYS
61	BD	21	ARG
61	BD	62	ARG
62	Ay	38	ARG
62	Ay	51	TRP
63	Ag	43	ARG
63	Ag	48	TYR
63	Ag	167	ASP
64	Ax	57	THR
64	Ax	63	TRP

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Mol	Chain	Res	Type
64	Ax	109	ASP
64	Ax	134	GLN
64	Ax	136	TYR
64	Ax	146	TRP
64	Ax	173	ARG
64	Ax	180	ARG
64	Ax	203	ARG
65	BL	107	TRP
65	BL	119	ARG
65	BL	132	HIS
65	BL	134	ARG
65	BL	141	TRP
65	BL	211	THR
65	BL	328	THR
66	BO	105	ARG
66	BO	125	ILE
66	BO	128	VAL
66	BO	148	ASP
66	BO	172	ARG
67	BG	1282	THR
67	BG	1284	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (307) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	162	GLN
1	A	184	ASN
1	A	207	HIS
1	A	337	ASN
2	B	74	GLN
2	B	88	GLN
2	B	133	GLN
2	B	153	ASN
2	B	170	HIS
2	B	172	HIS
2	B	177	HIS
2	B	200	ASN
2	B	273	ASN
2	B	276	ASN
2	B	306	GLN
2	B	323	HIS

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Mol	Chain	Res	Type
3	C	67	ASN
3	C	120	ASN
3	C	142	ASN
4	D	26	HIS
4	D	38	HIS
5	E	52	ASN
5	E	221	HIS
5	E	224	GLN
5	E	246	ASN
5	E	280	GLN
6	F	25	HIS
6	F	135	HIS
6	F	161	GLN
7	G	15	HIS
7	G	19	GLN
7	G	29	GLN
7	G	38	ASN
7	G	89	GLN
7	G	143	GLN
7	G	202	ASN
7	G	277	GLN
7	G	300	GLN
7	G	310	HIS
7	G	319	HIS
8	H	19	HIS
8	H	61	GLN
8	H	108	ASN
8	H	134	ASN
8	H	152	GLN
9	I	65	HIS
9	I	99	HIS
9	I	223	HIS
9	I	242	HIS
9	I	259	HIS
10	J	52	GLN
10	J	99	ASN
11	K	46	GLN
11	K	65	ASN
11	K	73	HIS
11	K	78	GLN
11	K	79	HIS
11	K	98	GLN

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Mol	Chain	Res	Type
11	K	101	GLN
11	K	145	HIS
12	L	14	GLN
12	L	29	ASN
12	L	30	HIS
12	L	52	GLN
13	M	19	GLN
13	M	24	GLN
13	M	31	HIS
13	M	76	ASN
13	M	131	GLN
13	M	173	HIS
13	M	230	HIS
14	N	58	ASN
14	N	77	ASN
15	O	23	GLN
15	O	89	HIS
15	O	104	GLN
15	O	187	GLN
15	O	212	HIS
15	O	296	HIS
15	O	303	GLN
15	O	306	ASN
15	O	314	GLN
16	P	61	GLN
17	Q	24	HIS
17	Q	170	ASN
18	R	23	ASN
18	R	67	HIS
18	R	71	HIS
18	R	167	HIS
18	R	194	GLN
18	R	246	ASN
18	R	286	GLN
18	R	370	GLN
18	R	419	GLN
18	R	421	ASN
18	R	470	HIS
19	S	256	ASN
19	S	312	GLN
19	S	327	HIS
19	S	336	GLN

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Mol	Chain	Res	Type
19	S	371	HIS
19	S	384	HIS
19	S	385	HIS
19	S	388	GLN
21	U	37	ASN
21	U	78	GLN
22	V	29	GLN
22	V	119	GLN
23	W	60	HIS
23	W	72	HIS
23	W	79	HIS
23	W	97	ASN
24	X	64	HIS
24	X	257	ASN
24	X	288	ASN
24	X	344	GLN
24	X	479	GLN
24	X	491	GLN
25	Y	149	GLN
25	Y	153	GLN
25	Y	231	GLN
25	Y	279	HIS
25	Y	282	GLN
26	Z	13	HIS
26	Z	14	ASN
26	Z	67	ASN
26	Z	91	ASN
26	Z	146	GLN
27	BA	91	HIS
29	BB	41	HIS
29	BB	55	GLN
29	BB	108	GLN
30	Aw	79	HIS
30	Aw	89	HIS
31	Bj	4	ASN
31	Bj	91	ASN
32	An	24	HIS
32	An	48	HIS
32	An	50	HIS
32	An	60	ASN
32	An	123	GLN
32	An	166	ASN

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Mol	Chain	Res	Type
32	An	212	HIS
32	An	221	GLN
32	An	238	GLN
32	An	240	GLN
32	An	264	HIS
32	An	295	HIS
32	An	314	HIS
33	Al	133	GLN
33	Al	250	GLN
33	Al	276	GLN
33	Al	279	ASN
33	Al	298	ASN
34	BI	81	HIS
34	BI	148	ASN
35	Az	19	GLN
35	Az	31	ASN
35	Az	70	HIS
35	Az	73	HIS
35	Az	128	GLN
36	At	28	ASN
36	At	33	ASN
36	At	56	ASN
36	At	73	HIS
36	At	90	GLN
37	BC	22	HIS
37	BC	63	ASN
37	BC	67	ASN
37	BC	90	GLN
37	BC	119	GLN
37	BC	123	ASN
38	Ab	10	GLN
38	Ab	27	GLN
38	Ab	37	HIS
38	Ab	84	HIS
38	Ab	94	ASN
38	Ab	205	HIS
38	Ab	245	GLN
38	Ab	257	GLN
39	Ai	64	GLN
39	Ai	142	ASN
39	Ai	151	ASN
39	Ai	184	HIS

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Mol	Chain	Res	Type
39	Ai	245	ASN
39	Ai	248	ASN
39	Ai	470	ASN
40	Ap	17	HIS
40	Ap	81	HIS
40	Ap	123	HIS
41	Au	74	GLN
41	Au	93	HIS
41	Au	99	HIS
41	Au	157	GLN
41	Au	167	HIS
42	Aa	20	GLN
42	Aa	109	HIS
42	Aa	112	HIS
42	Aa	159	GLN
42	Aa	194	ASN
43	Ao	90	HIS
43	Ao	248	GLN
43	Ao	271	GLN
43	Ao	280	ASN
44	BM	35	GLN
44	BM	113	GLN
44	BM	130	GLN
44	BM	228	ASN
44	BM	314	GLN
44	BM	325	GLN
44	BM	381	ASN
45	Ar	48	GLN
45	Ar	114	GLN
45	Ar	164	HIS
45	Ar	186	ASN
45	Ar	194	HIS
46	Aj	122	ASN
46	Aj	242	HIS
46	Aj	281	GLN
46	Aj	375	GLN
46	Aj	409	HIS
46	Aj	440	GLN
46	Aj	450	ASN
46	Aj	468	HIS
47	BH	82	HIS
47	BH	132	HIS

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Mol	Chain	Res	Type
47	BH	137	GLN
47	BH	149	ASN
47	BH	214	HIS
48	Am	15	HIS
48	Am	106	HIS
48	Am	144	HIS
48	Am	148	ASN
48	Am	152	GLN
48	Am	184	ASN
48	Am	228	GLN
48	Am	263	HIS
48	Am	278	GLN
48	Am	307	ASN
48	Am	315	ASN
49	Aq	19	HIS
49	Aq	36	HIS
49	Aq	55	ASN
49	Aq	109	HIS
49	Aq	281	GLN
49	Aq	308	GLN
51	Ak	22	HIS
51	Ak	64	GLN
51	Ak	93	HIS
51	Ak	216	HIS
51	Ak	294	GLN
52	BP	6	HIS
52	BP	49	GLN
53	Ad	85	GLN
53	Ad	187	GLN
53	Ad	220	ASN
53	Ad	230	HIS
55	Av	137	GLN
55	Av	168	HIS
56	Af	20	HIS
56	Af	100	GLN
56	Af	105	GLN
58	Ae	54	ASN
58	Ae	79	GLN
58	Ae	83	HIS
59	Ac	55	HIS
59	Ac	57	HIS
59	Ac	124	GLN

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Mol	Chain	Res	Type
59	Ac	132	GLN
59	Ac	147	GLN
59	Ac	245	GLN
60	Ah	107	HIS
60	Ah	184	HIS
60	Ah	200	GLN
60	Ah	272	GLN
60	Ah	347	ASN
60	Ah	385	GLN
61	BD	3	ASN
61	BD	48	GLN
61	BD	80	GLN
62	Ay	83	ASN
62	Ay	158	GLN
63	Ag	197	HIS
63	Ag	226	GLN
64	Ax	66	GLN
64	Ax	85	HIS
64	Ax	183	HIS
64	Ax	188	ASN
65	BL	84	GLN
65	BL	92	GLN
65	BL	118	HIS
65	BL	152	GLN
65	BL	224	HIS
65	BL	232	HIS
65	BL	284	ASN
65	BL	305	HIS
65	BL	335	HIS
65	BL	374	ASN
66	BO	118	HIS
66	BO	124	ASN
66	BO	137	ASN
66	BO	144	GLN
66	BO	176	HIS
67	BG	1274	ASN
67	BG	1328	GLN
67	BG	1336	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
71	1	1085/9070 (11%)	638 (58%)	127 (11%)

All (638) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
71	1	39	U
71	1	40	C
71	1	41	A
71	1	42	A
71	1	43	A
71	1	44	G
71	1	45	U
71	1	46	U
71	1	47	A
71	1	48	U
71	1	49	U
71	1	50	A
71	1	51	U
71	1	52	U
71	1	53	A
71	1	58	A
71	1	59	U
71	1	62	U
71	1	63	G
71	1	64	A
71	1	66	U
71	1	67	U
71	1	68	U
71	1	69	G
71	1	70	G
71	1	71	A
71	1	72	U
71	1	73	G
71	1	74	A
71	1	75	A
71	1	76	U
71	1	79	A
71	1	81	U
71	1	83	U
71	1	84	U
71	1	88	U
71	1	89	U
71	1	90	A

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Mol	Chain	Res	Type
71	1	91	U
71	1	92	A
71	1	93	U
71	1	96	U
71	1	98	G
71	1	99	A
71	1	102	U
71	1	103	U
71	1	104	U
71	1	106	A
71	1	107	U
71	1	108	U
71	1	110	U
71	1	111	A
71	1	113	U
71	1	115	U
71	1	116	U
71	1	117	U
71	1	118	U
71	1	119	G
71	1	120	A
71	1	126	U
71	1	127	A
71	1	128	U
71	1	130	U
71	1	132	U
71	1	134	A
71	1	135	A
71	1	136	A
71	1	137	U
71	1	138	A
71	1	139	U
71	1	141	A
71	1	142	U
71	1	143	A
71	1	144	U
71	1	145	A
71	1	146	U
71	1	147	U
71	1	148	U
71	1	149	U
71	1	150	A

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Mol	Chain	Res	Type
71	1	152	A
71	1	153	U
71	1	154	U
71	1	155	U
71	1	156	A
71	1	158	A
71	1	160	U
71	1	161	U
71	1	162	G
71	1	163	U
71	1	164	U
71	1	165	G
71	1	166	U
71	1	167	U
71	1	184	G
71	1	185	U
71	1	187	U
71	1	188	A
71	1	189	U
71	1	190	A
71	1	192	A
71	1	193	U
71	1	198	A
71	1	201	U
71	1	202	A
71	1	203	A
71	1	204	U
71	1	205	U
71	1	206	U
71	1	207	G
71	1	208	U
71	1	209	U
71	1	210	U
71	1	211	U
71	1	212	A
71	1	214	U
71	1	215	U
71	1	221	U
71	1	225	U
71	1	226	A
71	1	230	A
71	1	233	G

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Mol	Chain	Res	Type
71	1	238	U
71	1	239	U
71	1	240	A
71	1	241	U
71	1	245	U
71	1	246	U
71	1	247	A
71	1	249	U
71	1	250	A
71	1	251	U
71	1	252	U
71	1	253	U
71	1	254	U
71	1	256	A
71	1	257	G
71	1	259	U
71	1	268	A
71	1	270	A
71	1	271	U
71	1	272	A
71	1	280	A
71	1	282	U
71	1	283	G
71	1	284	A
71	1	285	U
71	1	286	G
71	1	287	G
71	1	288	C
71	1	289	A
71	1	290	C
71	1	292	G
71	1	293	U
71	1	294	U
71	1	298	C
71	1	299	U
71	1	300	A
71	1	301	U
71	1	302	A
71	1	303	U
71	1	304	G
71	1	306	A
71	1	307	C

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Mol	Chain	Res	Type
71	1	308	C
71	1	309	U
71	1	310	A
71	1	311	U
71	1	312	A
71	1	314	A
71	1	316	A
71	1	317	A
71	1	319	A
71	1	320	G
71	1	322	A
71	1	323	A
71	1	327	U
71	1	328	A
71	1	329	U
71	1	331	U
71	1	333	A
71	1	336	U
71	1	339	A
71	1	343	A
71	1	344	U
71	1	345	A
71	1	346	A
71	1	347	A
71	1	350	A
71	1	359	C
71	1	360	U
71	1	361	A
71	1	362	A
71	1	363	U
71	1	364	U
71	1	365	U
71	1	370	U
71	1	374	U
71	1	377	U
71	1	379	U
71	1	380	G
71	1	381	A
71	1	382	A
71	1	383	A
71	1	384	A
71	1	388	U

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Mol	Chain	Res	Type
71	1	391	A
71	1	392	A
71	1	393	A
71	1	394	U
71	1	396	A
71	1	397	A
71	1	398	U
71	1	399	U
71	1	400	U
71	1	401	U
71	1	402	U
71	1	404	U
71	1	405	U
71	1	407	C
71	1	411	U
71	1	412	U
71	1	413	U
71	1	414	U
71	1	415	U
71	1	416	A
71	1	418	A
71	1	420	A
71	1	421	U
71	1	422	U
71	1	423	G
71	1	424	A
71	1	425	A
71	1	426	G
71	1	427	U
71	1	429	A
71	1	431	A
71	1	432	U
71	1	433	G
71	1	434	U
71	1	435	A
71	1	439	A
71	1	440	A
71	1	443	G
71	1	446	U
71	1	447	A
71	1	449	U
71	1	450	A

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Mol	Chain	Res	Type
71	1	451	A
71	1	452	A
71	1	453	A
71	1	454	A
71	1	455	U
71	1	456	A
71	1	457	C
71	1	458	A
71	1	459	A
71	1	460	A
71	1	465	A
71	1	466	U
71	1	468	U
71	1	471	A
71	1	472	A
71	1	473	U
71	1	474	U
71	1	475	A
71	1	476	A
71	1	477	U
71	1	478	A
71	1	479	A
71	1	480	A
71	1	481	U
71	1	482	C
71	1	483	U
71	1	484	A
71	1	486	U
71	1	488	U
71	1	489	A
71	1	492	U
71	1	495	A
71	1	496	U
71	1	497	A
71	1	498	G
71	1	500	U
71	1	501	G
71	1	504	U
71	1	506	A
71	1	507	U
71	1	508	G
71	1	509	U

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Mol	Chain	Res	Type
71	1	510	U
71	1	511	A
71	1	512	A
71	1	514	U
71	1	515	A
71	1	516	A
71	1	517	U
71	1	518	U
71	1	519	U
71	1	520	A
71	1	521	U
71	1	522	U
71	1	523	A
71	1	524	U
71	1	525	U
71	1	526	U
71	1	527	U
71	1	528	A
71	1	529	A
71	1	532	U
71	1	536	A
71	1	537	U
71	1	538	A
71	1	543	U
71	1	544	U
71	1	545	U
71	1	546	A
71	1	547	U
71	1	548	A
71	1	549	C
71	1	550	A
71	1	552	A
71	1	555	U
71	1	556	A
71	1	557	A
71	1	558	C
71	1	559	U
71	1	560	U
71	1	561	U
71	1	562	U
71	1	564	U
71	1	565	U

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Mol	Chain	Res	Type
71	1	566	G
71	1	567	A
71	1	568	A
71	1	572	A
71	1	573	A
71	1	574	A
71	1	575	G
71	1	576	A
71	1	578	U
71	1	580	A
71	1	581	U
71	1	582	U
71	1	583	A
71	1	584	U
71	1	587	U
71	1	588	A
71	1	589	A
71	1	591	U
71	1	592	A
71	1	593	U
71	1	594	U
71	1	595	A
71	1	596	U
71	1	597	U
71	1	598	U
71	1	599	U
71	1	600	A
71	1	601	A
71	1	602	A
71	1	604	A
71	1	608	A
71	1	609	A
71	1	612	A
71	1	617	G
71	1	618	U
71	1	621	A
71	1	622	U
71	1	624	A
71	1	625	A
71	1	626	A
71	1	627	U
71	1	629	A

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Mol	Chain	Res	Type
71	1	630	U
71	1	631	C
71	1	632	A
71	1	633	A
71	1	634	G
71	1	641	A
71	1	642	A
71	1	643	G
71	1	644	C
71	1	645	G
71	1	647	U
71	1	648	U
71	1	649	A
71	1	650	U
71	1	651	U
71	1	652	A
71	1	653	A
71	1	655	U
71	1	661	G
71	1	665	U
71	1	666	A
71	1	667	A
71	1	668	G
71	1	669	U
71	1	670	A
71	1	675	A
71	1	679	A
71	1	680	A
71	1	684	U
71	1	685	A
71	1	690	U
71	1	691	G
71	1	697	A
71	1	698	G
71	1	699	A
71	1	700	U
71	1	701	U
71	1	702	U
71	1	704	U
71	1	705	A
71	1	710	A
71	1	712	U

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Mol	Chain	Res	Type
71	1	749	U
71	1	750	U
71	1	751	A
71	1	754	A
71	1	755	G
71	1	756	U
71	1	760	A
71	1	763	G
71	1	764	U
71	1	765	A
71	1	768	U
71	1	769	U
71	1	772	U
71	1	775	C
71	1	776	U
71	1	781	A
71	1	782	U
71	1	783	U
71	1	784	A
71	1	785	A
71	1	786	A
71	1	787	G
71	1	788	C
71	1	789	G
71	1	790	U
71	1	791	U
71	1	794	A
71	1	795	U
71	1	796	A
71	1	798	A
71	1	799	A
71	1	802	U
71	1	807	A
71	1	808	A
71	1	809	A
71	1	810	U
71	1	811	U
71	1	812	A
71	1	813	U
71	1	815	A
71	1	816	C
71	1	817	A

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Mol	Chain	Res	Type
71	1	821	U
71	1	822	A
71	1	830	A
71	1	835	A
71	1	836	U
71	1	837	U
71	1	839	A
71	1	845	A
71	1	847	A
71	1	848	U
71	1	850	U
71	1	851	U
71	1	857	A
71	1	858	A
71	1	859	U
71	1	860	U
71	1	863	A
71	1	864	A
71	1	868	U
71	1	869	A
71	1	870	A
71	1	873	U
71	1	876	G
71	1	887	C
71	1	888	U
71	1	889	C
71	1	890	U
71	1	892	C
71	1	893	U
71	1	894	U
71	1	895	U
71	1	896	A
71	1	902	A
71	1	903	G
71	1	904	A
71	1	905	A
71	1	906	C
71	1	907	G
71	1	908	U
71	1	910	U
71	1	911	A
71	1	914	U

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Mol	Chain	Res	Type
71	1	915	G
71	1	916	U
71	1	917	A
71	1	918	A
71	1	919	U
71	1	924	U
71	1	925	G
71	1	927	U
71	1	928	U
71	1	929	G
71	1	930	A
71	1	933	G
71	1	934	G
71	1	939	A
71	1	940	U
71	1	941	A
71	1	943	U
71	1	944	A
71	1	945	U
71	1	948	C
71	1	949	U
71	1	952	U
71	1	953	U
71	1	954	A
71	1	955	U
71	1	960	A
71	1	961	A
71	1	962	A
71	1	963	A
71	1	964	A
71	1	969	U
71	1	971	U
71	1	972	A
71	1	973	U
71	1	974	U
71	1	975	U
71	1	977	U
71	1	978	U
71	1	980	A
71	1	982	A
71	1	983	U
71	1	984	A

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Mol	Chain	Res	Type
71	1	985	A
71	1	988	A
71	1	990	A
71	1	992	G
71	1	993	U
71	1	995	C
71	1	996	G
71	1	997	A
71	1	998	G
71	1	999	C
71	1	1002	G
71	1	1003	U
71	1	1004	U
71	1	1005	A
71	1	1006	A
71	1	1007	C
71	1	1008	A
71	1	1009	A
71	1	1010	G
71	1	1011	C
71	1	1012	A
71	1	1013	U
71	1	1014	U
71	1	1015	A
71	1	1016	A
71	1	1017	U
71	1	1018	A
71	1	1019	C
71	1	1025	G
71	1	1028	U
71	1	1031	C
71	1	1032	A
71	1	1033	U
71	1	1034	C
71	1	1035	G
71	1	1036	U
71	1	1037	C
71	1	1038	U
71	1	1040	C
71	1	1041	U
71	1	1044	U
71	1	1045	U

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Mol	Chain	Res	Type
71	1	1046	G
71	1	1047	C
71	1	1050	A
71	1	1051	A
71	1	1053	U
71	1	1054	A
71	1	1055	U
71	1	1056	A
71	1	1059	U
71	1	1062	U
71	1	1063	U
71	1	1064	G
71	1	1065	U
71	1	1066	U
71	1	1068	A
71	1	1069	U
71	1	1072	A
71	1	1073	A
71	1	1074	A
71	1	1075	A
71	1	1086	U
71	1	1093	G
71	1	1095	U
71	1	1096	A
71	1	1097	A
71	1	1098	A
71	1	1099	A
71	1	1100	U
71	1	1101	C
71	1	1103	U
71	1	1105	G
71	1	1107	A
71	1	1111	C
71	1	1116	U
71	1	1117	U
71	1	1118	G
71	1	1122	A
71	1	1123	U
71	1	1124	A
71	1	1125	U
71	1	1126	A
71	1	1127	U

Continued on next page...

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Mol	Chain	Res	Type
71	1	1128	U
71	1	1129	U
71	1	1135	U
71	1	1136	U
71	1	1137	G
71	1	1138	U
71	1	1139	A
71	1	1140	U
71	1	1141	A
71	1	1146	U
71	1	1157	A
71	1	1158	U

All (127) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
71	1	39	U
71	1	40	C
71	1	41	A
71	1	45	U
71	1	47	A
71	1	50	A
71	1	65	U
71	1	70	G
71	1	74	A
71	1	97	U
71	1	98	G
71	1	106	A
71	1	131	U
71	1	135	A
71	1	146	U
71	1	155	U
71	1	161	U
71	1	164	U
71	1	191	A
71	1	201	U
71	1	202	A
71	1	203	A
71	1	204	U
71	1	206	U
71	1	207	G
71	1	208	U

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Mol	Chain	Res	Type
71	1	209	U
71	1	210	U
71	1	239	U
71	1	249	U
71	1	269	A
71	1	282	U
71	1	284	A
71	1	293	U
71	1	299	U
71	1	303	U
71	1	309	U
71	1	343	A
71	1	346	A
71	1	369	A
71	1	381	A
71	1	398	U
71	1	401	U
71	1	403	U
71	1	406	U
71	1	412	U
71	1	413	U
71	1	414	U
71	1	416	A
71	1	424	A
71	1	430	U
71	1	433	G
71	1	450	A
71	1	455	U
71	1	477	U
71	1	487	U
71	1	491	U
71	1	506	A
71	1	508	G
71	1	509	U
71	1	511	A
71	1	513	U
71	1	519	U
71	1	523	A
71	1	547	U
71	1	565	U
71	1	572	A
71	1	592	A

Continued on next page...

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Mol	Chain	Res	Type
71	1	593	U
71	1	595	A
71	1	596	U
71	1	617	G
71	1	626	A
71	1	628	U
71	1	632	A
71	1	642	A
71	1	643	G
71	1	649	A
71	1	650	U
71	1	652	A
71	1	660	C
71	1	668	G
71	1	689	U
71	1	697	A
71	1	698	G
71	1	703	U
71	1	704	U
71	1	754	A
71	1	759	C
71	1	763	G
71	1	781	A
71	1	782	U
71	1	790	U
71	1	798	A
71	1	811	U
71	1	821	U
71	1	835	A
71	1	844	A
71	1	847	A
71	1	849	U
71	1	858	A
71	1	862	A
71	1	905	A
71	1	906	C
71	1	910	U
71	1	915	G
71	1	916	U
71	1	928	U
71	1	929	G
71	1	932	U

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Mol	Chain	Res	Type
71	1	944	A
71	1	951	U
71	1	960	A
71	1	974	U
71	1	1015	A
71	1	1044	U
71	1	1054	A
71	1	1067	C
71	1	1074	A
71	1	1097	A
71	1	1121	U
71	1	1122	A
71	1	1125	U
71	1	1126	A
71	1	1127	U
71	1	1128	U
71	1	1157	A

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
73	NAD	Ag	301	-	42,48,48	0.61	0	50,73,73	1.12	5 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
73	NAD	Ag	301	-	-	11/26/62/62	0/5/5/5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
73	Ag	301	NAD	O4D-C1D-C2D	-4.10	100.93	106.93
73	Ag	301	NAD	C3D-C2D-C1D	3.28	105.91	100.98
73	Ag	301	NAD	C6N-N1N-C2N	-2.20	119.97	121.97
73	Ag	301	NAD	C5A-C6A-N6A	2.15	123.62	120.35
73	Ag	301	NAD	O4B-C4B-C3B	-2.09	100.98	105.11

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
73	Ag	301	NAD	C5B-O5B-PA-O3
73	Ag	301	NAD	C2D-C1D-N1N-C2N
73	Ag	301	NAD	C4B-C5B-O5B-PA
73	Ag	301	NAD	PN-O3-PA-O5B
73	Ag	301	NAD	PA-O3-PN-O5D
73	Ag	301	NAD	C4D-C5D-O5D-PN
73	Ag	301	NAD	C5B-O5B-PA-O1A
73	Ag	301	NAD	PA-O3-PN-O1N
73	Ag	301	NAD	PN-O3-PA-O2A
73	Ag	301	NAD	C2D-C1D-N1N-C6N
73	Ag	301	NAD	C5D-O5D-PN-O1N

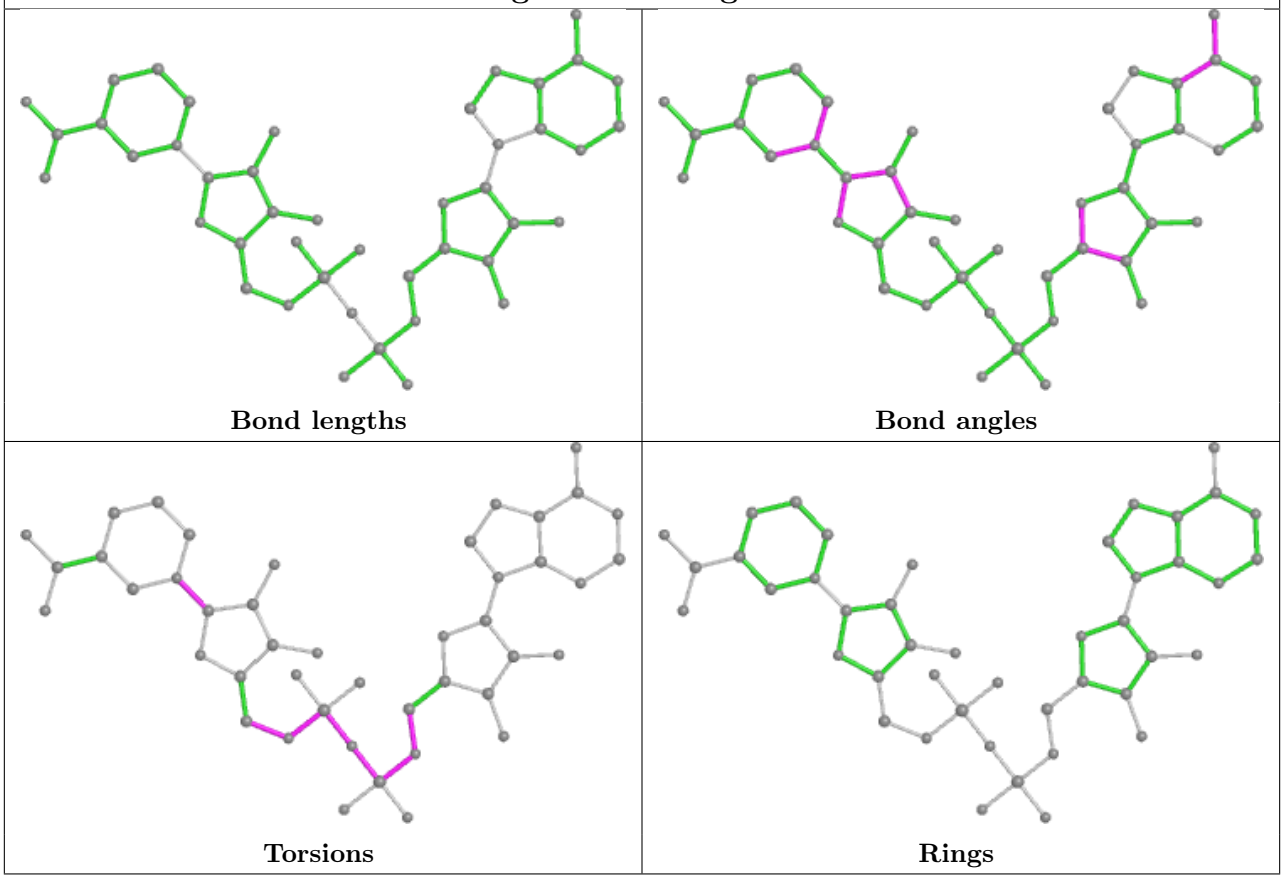
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAD Ag 301



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

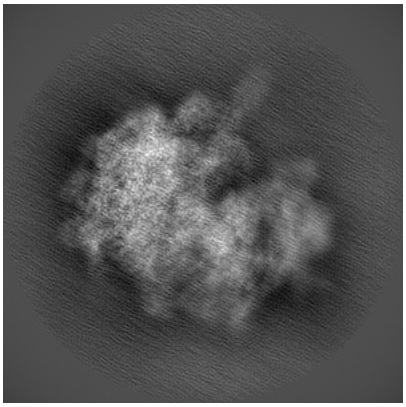
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11796. These allow visual inspection of the internal detail of the map and identification of artifacts.

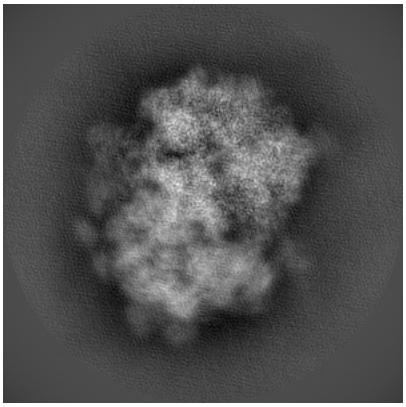
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

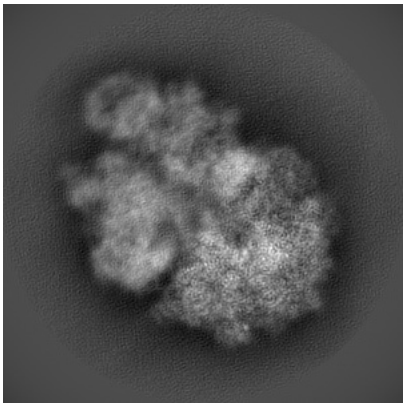
6.1.1 Primary map



X



Y

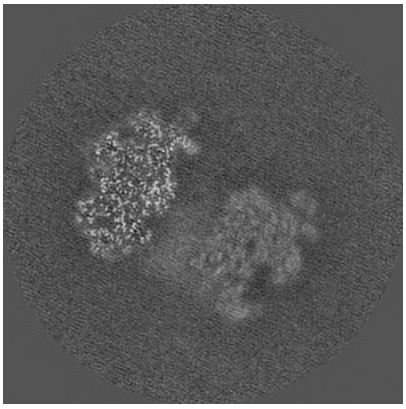


Z

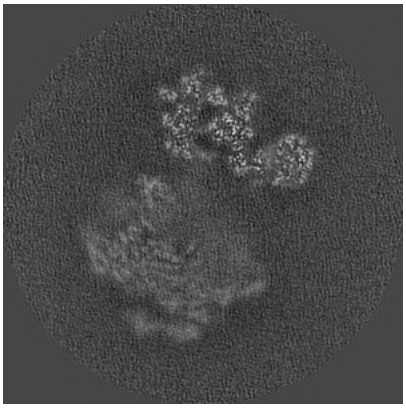
The images above show the map projected in three orthogonal directions.

6.2 Central slices

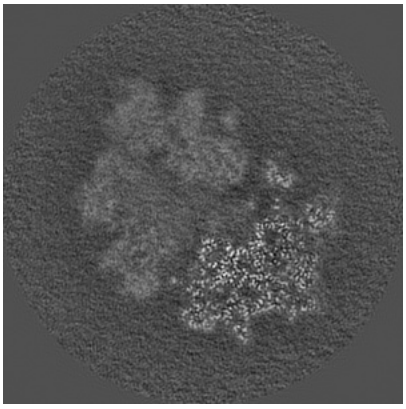
6.2.1 Primary map



X Index: 200



Y Index: 200

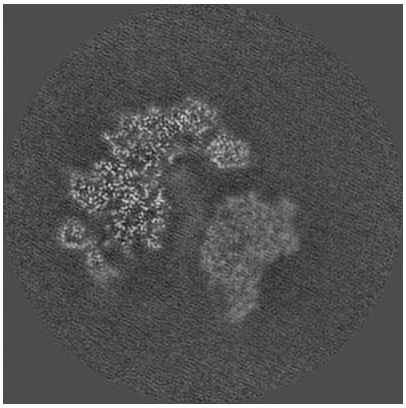


Z Index: 200

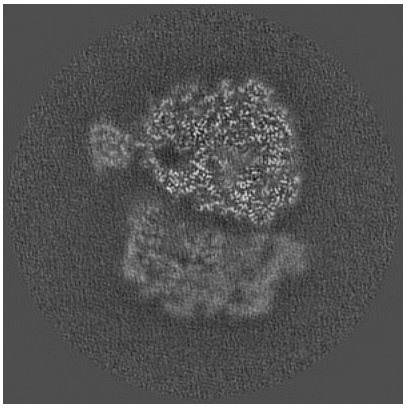
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

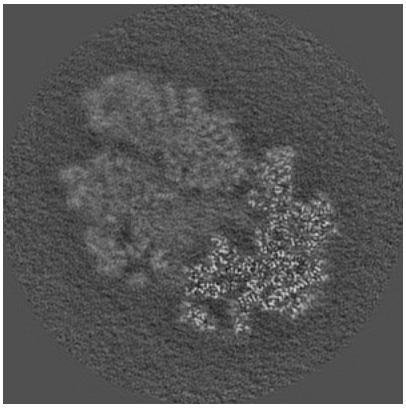
6.3.1 Primary map



X Index: 224



Y Index: 150



Z Index: 185

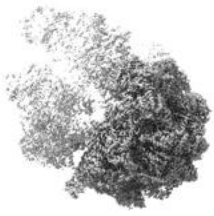
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

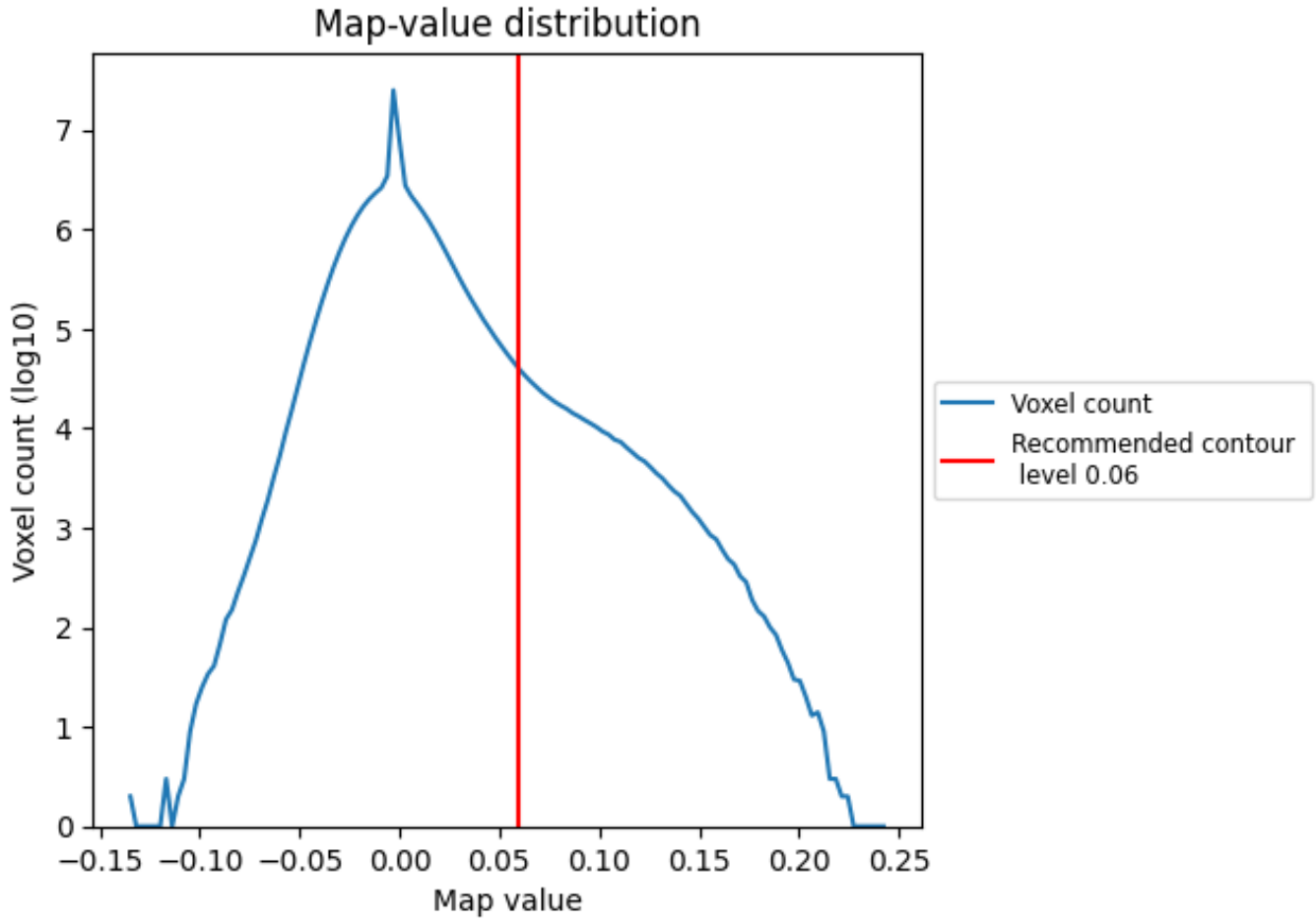
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

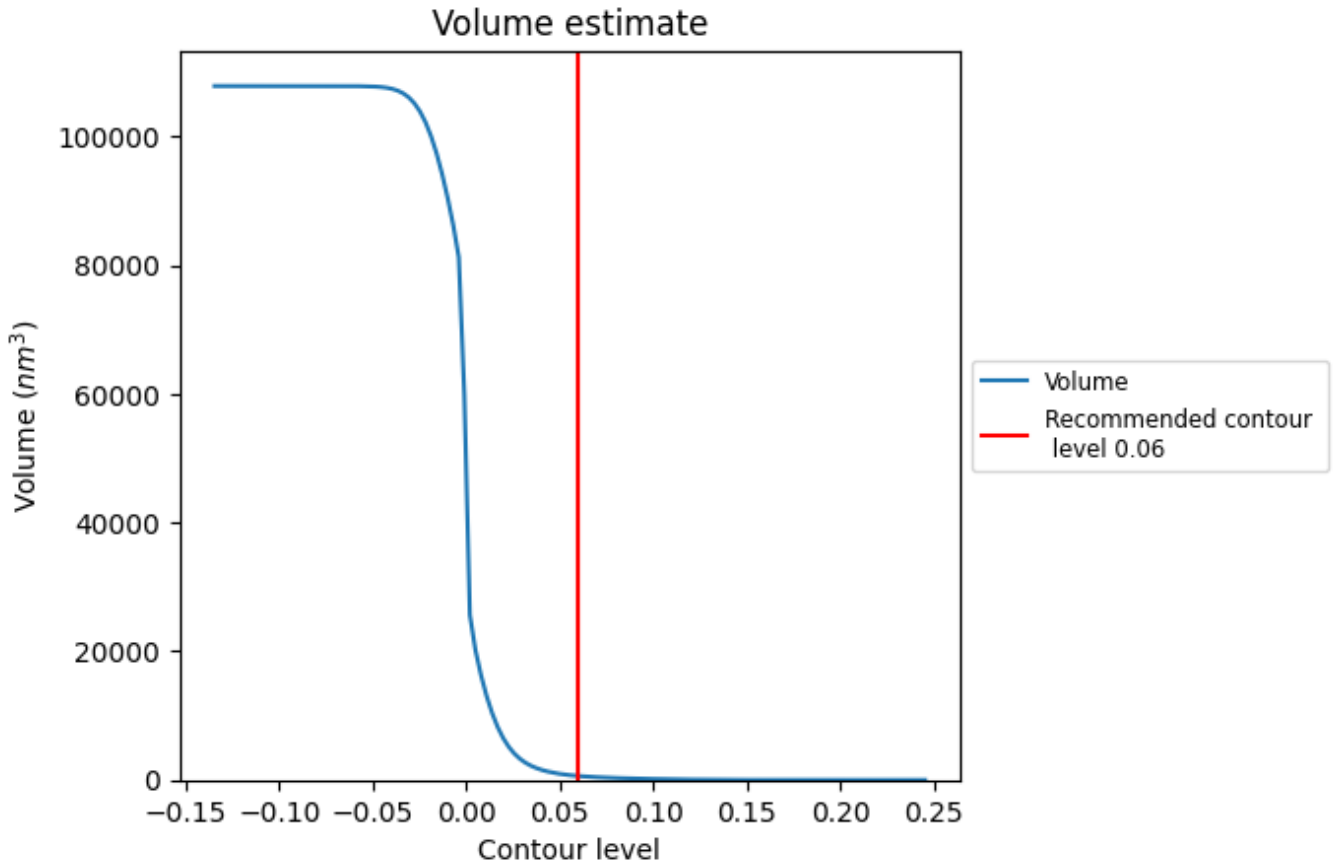
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

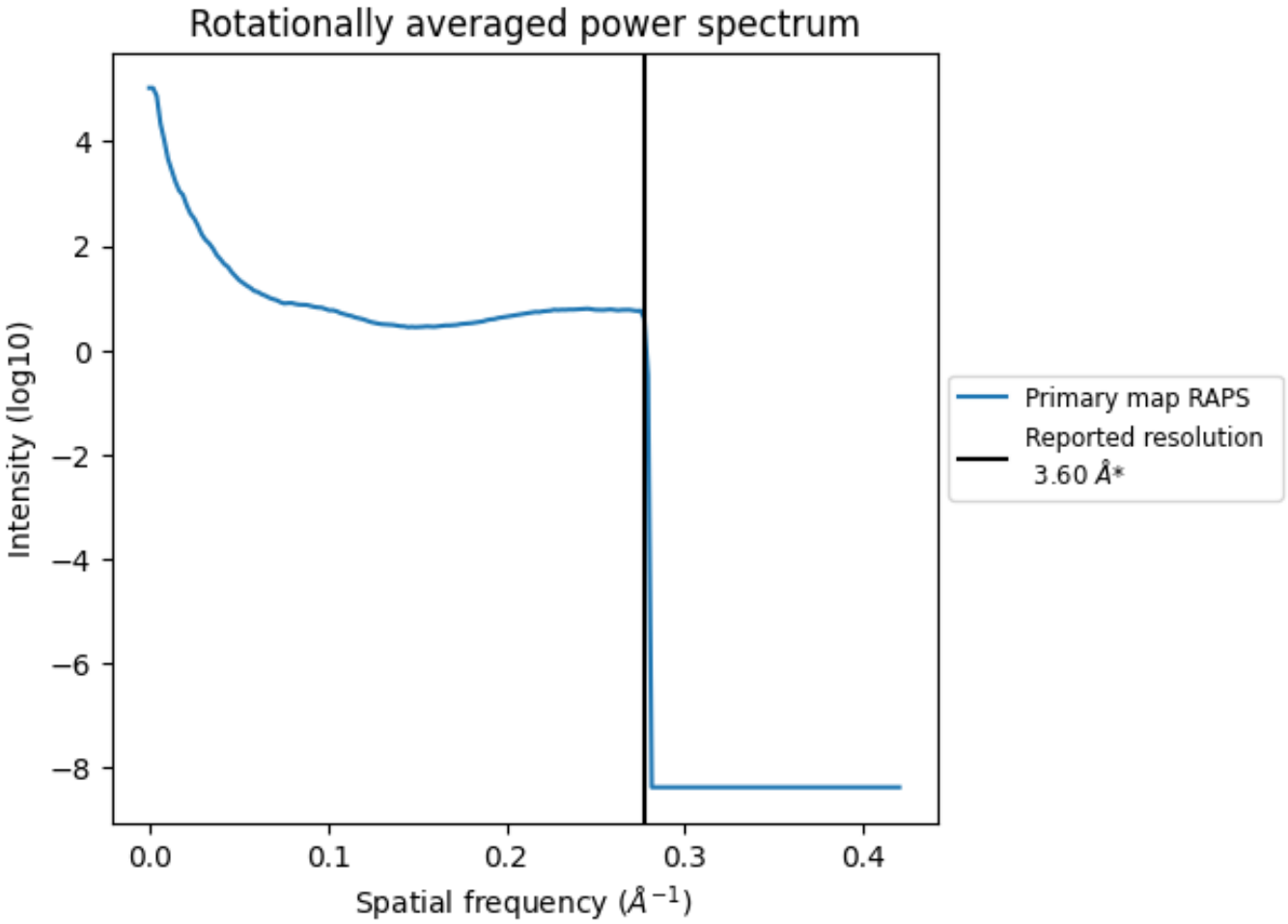
7.2 Volume estimate



The volume at the recommended contour level is 617 nm^3; this corresponds to an approximate mass of 557 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

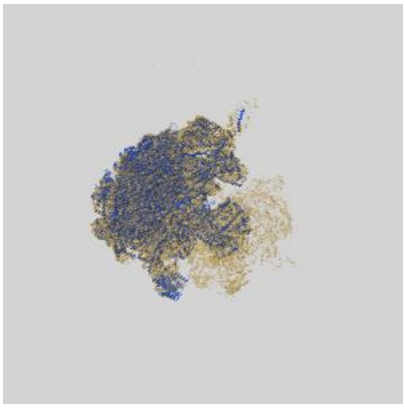
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

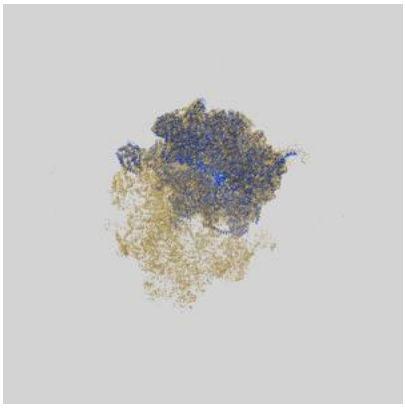
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11796 and PDB model 7AIH. Per-residue inclusion information can be found in section 3 on page 18.

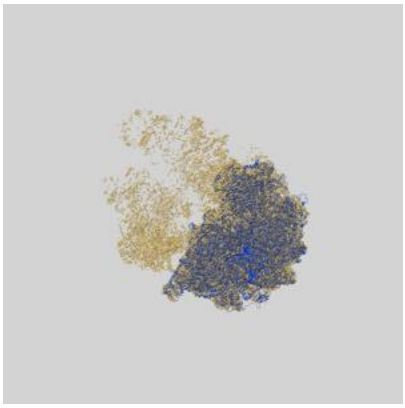
9.1 Map-model overlay



X



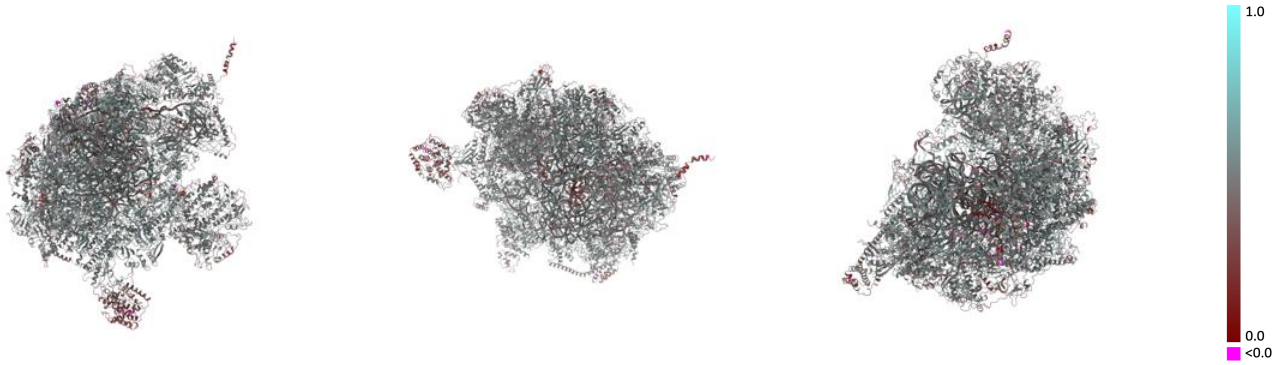
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

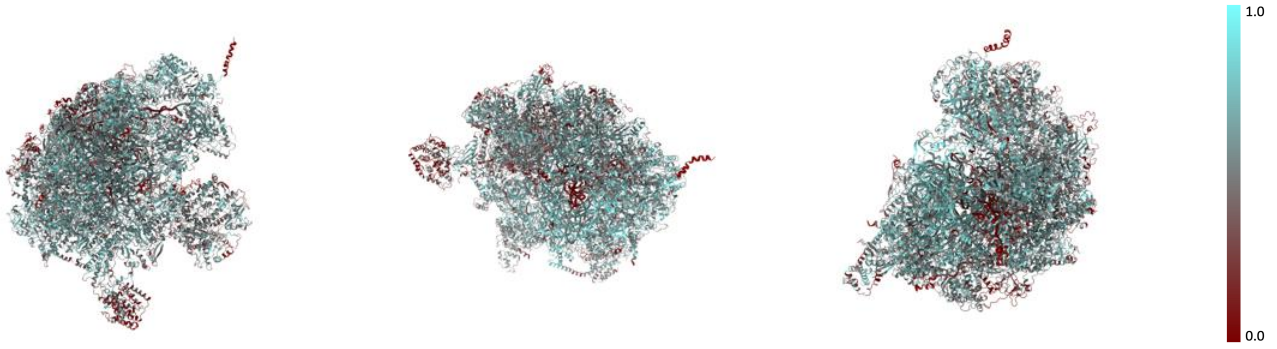
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

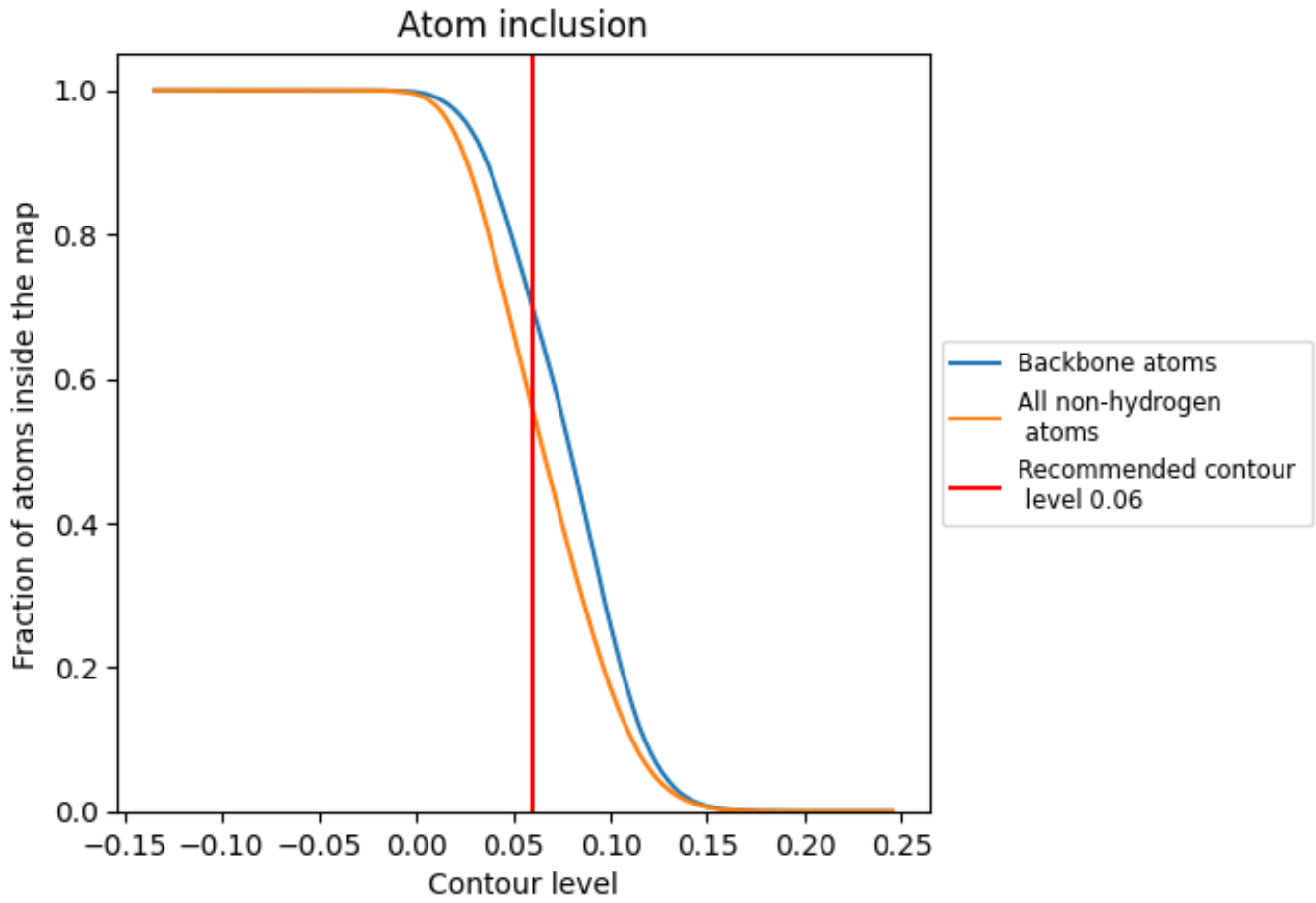
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5559	0.4790
1	0.6135	0.4520
A	0.6485	0.5200
Aa	0.4527	0.4490
Ab	0.6170	0.5000
Ac	0.4805	0.4600
Ad	0.5163	0.4950
Ae	0.6225	0.5110
Af	0.5225	0.4740
Ag	0.5739	0.5060
Ah	0.5277	0.4630
Ai	0.5569	0.5060
Aj	0.5566	0.4990
Ak	0.4718	0.4440
Al	0.5895	0.4970
Am	0.6382	0.4910
An	0.5486	0.4840
Ao	0.6244	0.5100
Ap	0.4922	0.4530
Aq	0.5037	0.5020
Ar	0.6093	0.5180
As	0.5424	0.4690
At	0.5907	0.4980
Au	0.6162	0.5040
Av	0.5245	0.4600
Aw	0.6012	0.4990
Ax	0.6048	0.4990
Ay	0.5883	0.4910
Az	0.6374	0.5210
B	0.5877	0.5130
BA	0.4916	0.4510
BB	0.5561	0.4620
BC	0.4968	0.4860
BD	0.6093	0.5130
BE	0.5691	0.4430

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Chain	Atom inclusion	Q-score
BF	0.4963	0.4800
BG	0.5609	0.4930
BH	0.5450	0.4970
BI	0.5760	0.4760
BL	0.5948	0.5110
BM	0.2679	0.3150
BO	0.5193	0.4600
BP	0.5468	0.4990
Bj	0.4445	0.4790
C	0.6005	0.5080
D	0.4773	0.4210
E	0.5621	0.4670
F	0.5609	0.5100
G	0.5959	0.5200
H	0.4929	0.4920
I	0.5467	0.4970
J	0.5653	0.4970
K	0.5551	0.4920
L	0.5848	0.5030
M	0.5721	0.5010
N	0.5678	0.4990
O	0.3662	0.4270
P	0.5374	0.5070
Q	0.5676	0.4970
R	0.5171	0.4670
S	0.5555	0.5110
T	0.6375	0.5140
U	0.4743	0.4910
UA	0.6621	0.4690
UB	0.6776	0.5100
UC	0.2806	0.3630
UD	0.5453	0.3890
V	0.5567	0.5230
W	0.5617	0.5070
X	0.5125	0.4770
Y	0.4661	0.4700
Z	0.5639	0.5010